

SEARCH REQUEST FORM

Requestor's

Name:

BERCH

Serial

Number:

03/26508

Date:

3/10/04

Phone:

571-272-0663

Art Unit:

1624

Office

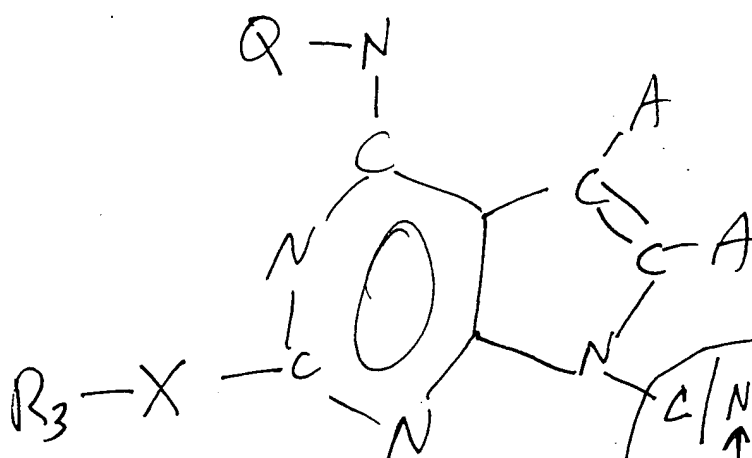
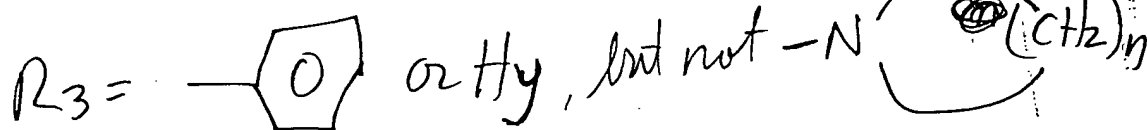
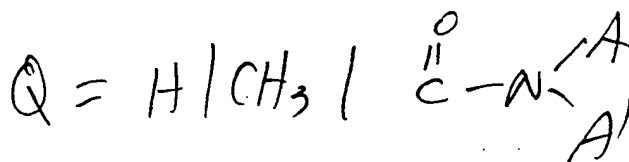
Perm 5001

Mailbox

5C18

Search Topic:

Please write a detailed statement of search topic. Describe specifically as possible the subject matter to be searched. Define any terms that may have a special meaning. Give examples or relevant citations, authors, keywords, etc., if known. For sequences, please attach a copy of the sequence. You may include a copy of the broadest and/or most relevant claim(s).


$$A, A' = H/CH_3:$$

$$n = 3 - 8$$
$$X = O/N/S/bond$$

~~If I get zero hits, let this be~~

STAFF USE ONLY

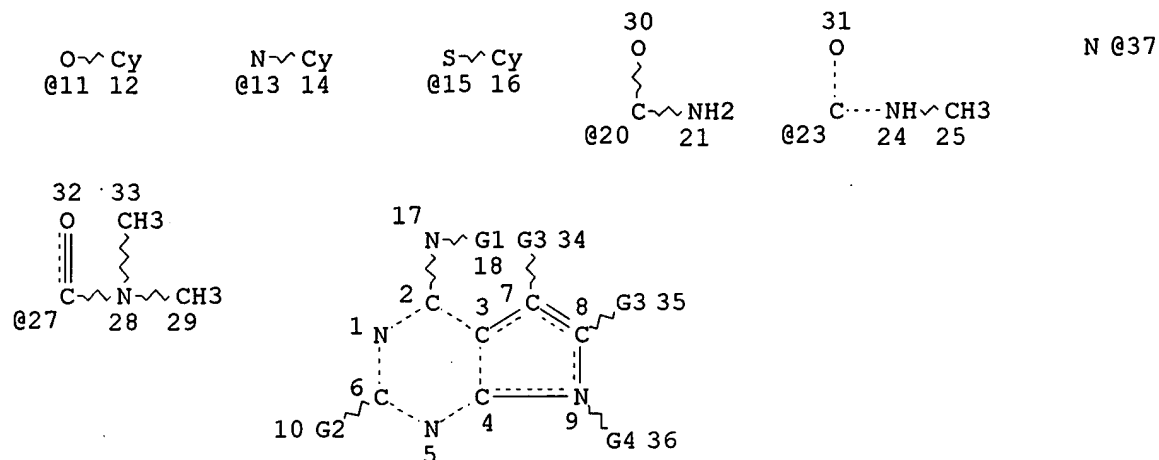
Date completed:

PCT/26508

(FILE 'REGISTRY' ENTERED AT 14:26:01 ON 12 MAR 2004)

L1

STR



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VAR G2=11/13/15/CY
VAR G3=H/CH3
VAR G4=C/37/H
NODE ATTRIBUTES:
NSPEC IS R AT 37
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 34

STEREO ATTRIBUTES: NONE
L2 249 SEA FILE=REGISTRY SSS FUL L1

100.0% PROCESSED 12153 ITERATIONS
SEARCH TIME: 00.00.01

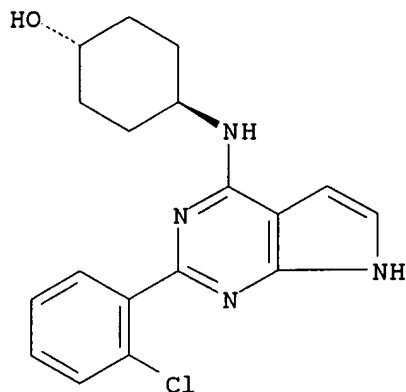
249 ANSWERS

=> d scan

L2 249 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Cyclohexanol, 4-[2-(2-chlorophenyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans- (9CI)
MF C18 H19 Cl N4 O

Relative stereochemistry.

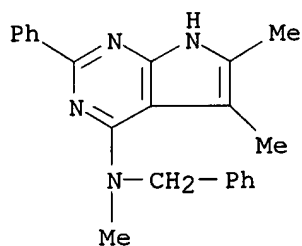
PCT/26508



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):5

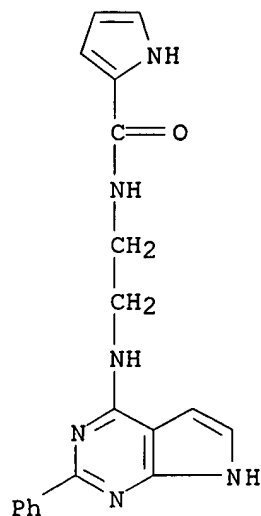
L2 249 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 1H-Pyrrolo[2,3-d]pyrimidin-4-amine, N,5,6-trimethyl-2-phenyl-N-(phenylmethyl)- (9CI)
MF C22 H22 N4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

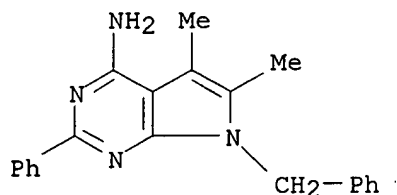
L2 249 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 1H-Pyrrolo[2,3-d]pyrimidin-4-amine, N-[2-[(2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]ethyl]- (9CI)
MF C19 H18 N6 O

PCT/26508



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

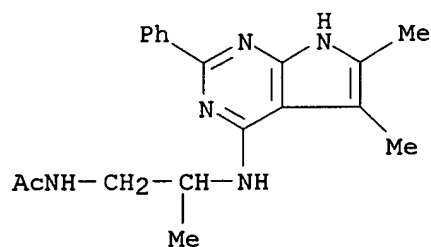
L2 249 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 7H-Pyrrolo[2,3-d]pyrimidin-4-amine, 5,6-dimethyl-2-phenyl-7-
(phenylmethyl)- (9CI)
MF C21 H20 N4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

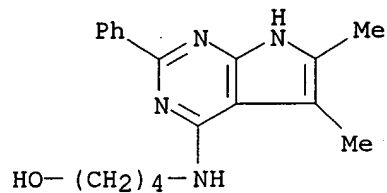
L2 249 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Acetamide, N-[2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-
yl)amino]propyl]- (9CI)
MF C19 H23 N5 O

PCT/26508



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 249 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 1-Butanol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]- (9CI)
MF C18 H22 N4 O



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

FILE 'HCAPLUS' ENTERED AT 14:29:08 ON 12 MAR 2004
L3 30 S L2

=> sel hit l3 1-30 rn
E1 THROUGH E245 ASSIGNED

FILE 'HOME' ENTERED AT 14:29:20 ON 12 MAR 2004

E0490133

2004 077 14:27:27

REQUEST NUMBER: P077138C

File Reg. @ 249 ans.

10525478

BEVERLY SHEARS
US PATENT & TRADEMARK OFFICE
BIOTECH/CHEM LIBRARY, RM 1A54
HENRY REMSEN, JR. BLDG.
400 DULANY ST.
ALEXANDRIA, VA 22314

CHEMICAL ABSTRACTS "REGISTRY FILE"

The REGISTRY File contains chemical substance records for substances identified by the CAS Registry System. The codes used to label the fields are shown below.

SUBSTANCE INFORMATION FIELD CODES

AF	Alternate Molecular Formula
AR	Alternate CAS Registry Number
CCI	Component Class Identifier
CCN	Condensed Chemical Name (all names)
CI	Class Identifier
CIL	Component Isotope at Unknown Location
CMF	Component Molecular Formula
CN	Chemical Name (up to 50)
COMP	Composition
CRN	Component CAS Registry Number
DEF	Definition
DR	Deleted CAS Registry Number
ENTE	Editor Note
FCN	All Chemical Names
FS	File Segment
IL	Isotope at Unknown Location
IN	CA Index Name
LC	CAS Registry Number Locator
MF	Molecular Formula
PCT	Polymer Class Term
PR	Preferred CAS Registry Number
REF	Number of References in CAPIUS, CA, and CAOLD, and the number of references in CA for the non-specific derivatives
RN	CAS Registry Number
RR	Replacing Registry Number
RSD	Ring System Data
SCN	Short Chemical Name (IN and OTHER NAMES)
SR	Source of Registration
SRSD	Short Ring System Data
STR	Structure Diagram with stereo bond and R/S/Z/E designations, if available

STF Flat Structure Diagram (no stereo bonds)
STS Structure Diagram with stereo bonds, if available

Sequence Field Codes:

NA Nucleic Acid
NTE Note
PNTE Patent Annotation
SEQ Sequence (1-letter amino acid codes)
SEQ3 Sequence (3-letter amino acid codes)
SQL Sequence Length

Property Field Codes:

BCF Bioconcentration Factor
BP Boiling Point
DEN Density
ECND Electric Conductivity
ECON Electric Conductance
ERES Electric Resistance
EREST Electric Resistivity
FP Flash Point
FRB Freely Rotable Bonds
HAC H acceptors
HD H donors
HVAP Enthalpy of Vaporization
KOC Organic Carbon Adsorption Coefficient
LD50 Median Lethal Dose
LOGD logD
LOGP logP
MM Magnetic Moment
MP Melting Point
MW Molecular Weight
ORP Optical Rotatory Power
PKA pKa
RI Refractive Index
SLB.MOL Molar Solubility
TG Glass Transition Temperature
TS Tensile Strength
VP Vapor Pressure

CA DOCUMENT REFERENCE FIELD CODES

AN	Accession Number
TI	Title of Document
AU	Author
IN	Patent Inventor
CS	Corporate Source
PA	Patent Assignee
SO	Source
PB	Publisher
PUI	Publisher Item Identifier
URL	Uniform Resource Locator
DT	Document Type
LA	Language
IC	International Patent Classification (IPC)
ICM	Main IPC
ICS	Secondary IPC
ICA	Additional or Supplementary IPC
ICI	Index or Complementary IPC
NCL	National Patent Classification Code
CC	Classification Code (CA Section Code and Title and CA Section Cross-Reference Code)
FAN.CNT	Family Accession Number Count
CY.CNT	Patent Country Count
PN.CNT	Patent Number Count
PI	Patent Information or Patent Family Table
DS	Designated States (patent)
AI	Patent Application Information
PRAI	Priority Application Information
PY	Publication Year
FAN	Family Accession Number
OS	Other Source
GI	Graphic Image
AB	Abstract
ST	Supplementary Term (CA Keywords)
IT	Index Term
RL	Role
REC.CNT	Cited References Count
RE	Cited References
RETABLE	Cited References Table

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REGISTRY FILE SEARCH STATISTICS - P077138C

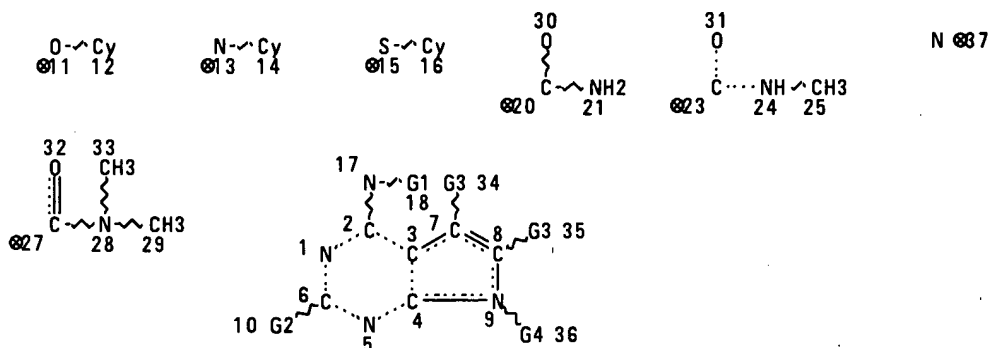
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4

249 ANSWERS PRINTED IN FORMAT 'IDE CAN'
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L1

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VAR G3=H/CH3

VAR G4=C/37/H

NODE ATTRIBUTES:

NSPEC IS R AT 37

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC I

NUMBER OF NODES IS 34

STEREO ATTRIBUTES: NONE

L2

249 SEA FILE=REGISTRY SSS FUL L1

100.0% PROCESSED 12153 ITERATIONS

249 ANSWERS

SEARCH TIME: 00.00.01

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REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE

5

L2 ANSWER 1 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 565234-92-6 REGISTRY

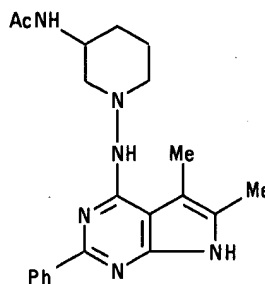
CN Acetamide, *N*-[1-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]-3-piperidiny]- (9CI)
(CA INDEX NAME)

FS 3D CONCORD

MF C₂₁H₂₆N₆O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

139:133575

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18 PAGE

6

L2 ANSWER 2 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 553634-53-0 REGISTRY

CN Acetamide,

N-[2-[[[6-methyl-7-[2-oxo-2-[4-(3-phenyl-2-propenyl)-1-piperazinyl]ethyl]-2-phenyl-7*H*-pyrrolo[2,3-*d*]-pyrimidin-4-yl]amino]ethyl]- (9CI) (CA INDEX NAME)

OTHER NAMES:

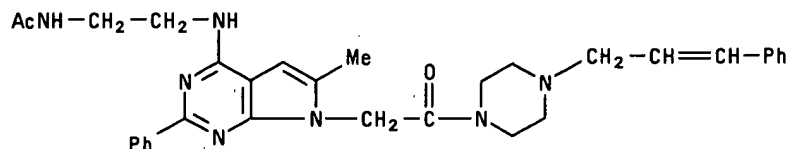
CN *N*-[2-[[[6-Methyl-7-[2-oxo-2-[4-(3-phenylallyl)piperazin-1-yl]ethyl]-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl]amino]ethyl]acetamide

FS 3D CONCORD

MF C₃₂H₃₇N₇O₂

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



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1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

139:85365

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REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE

7

L2 ANSWER 3 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 541503-91-7 REGISTRY

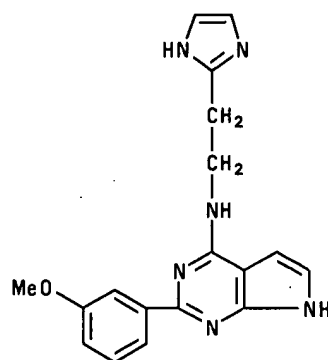
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, *N*-[2-(1*H*-imidazol-2-yl)ethyl]-2-(3-methoxyphenyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₁₈H₁₈N₆O

SR CA

LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

139:36534

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REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

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L2 ANSWER 4 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 541503-87-1 REGISTRY

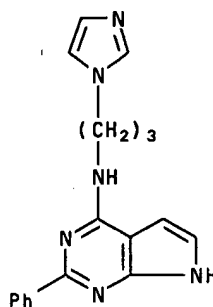
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, *N*-[3-(1*H*-imidazol-1-yl)propyl]-2-phenyl- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₁₈H₁₈N₆

SR CA

LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

139:36534

L2 ANSWER 5 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 541503-85-9 REGISTRY

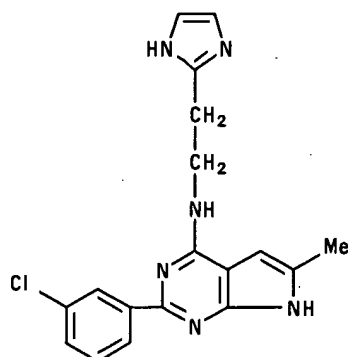
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 2-(3-chlorophenyl)-*N*-[2-(1*H*-imidazol-2-yl)ethyl]-6-methyl- (9CI)
(CA INDEX NAME)

FS 3D CONCORD

MF C₁₈H₁₇ClN₆

SR CA

LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

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STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

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10

L2 ANSWER 6 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 541503-83-7 REGISTRY

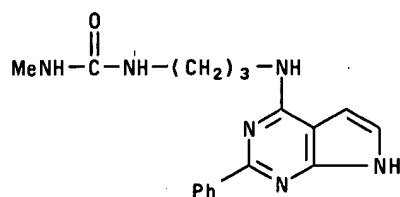
CN Urea, *N*-methyl-*N'*-[3-[(2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]propyl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₁₇H₂₀N₆O

SR CA

LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

139:36534

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

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PAGE 11

L2 ANSWER 7 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 541503-80-4 REGISTRY

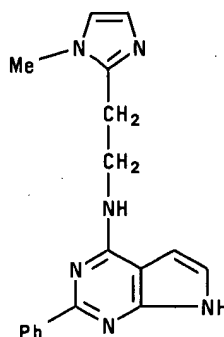
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, *N*-[2-(1-methyl-1*H*-imidazol-2-yl)ethyl]-2-phenyl- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₁₈H₁₈N₆

SR CA

LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

139:36534

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

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PAGE

12

L2 ANSWER 8 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 541503-77-9 REGISTRY

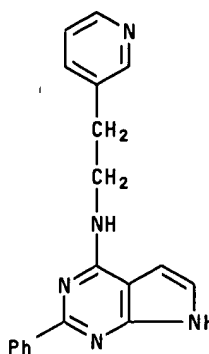
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 2-phenyl-*N*-[2-(3-pyridinyl)ethyl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₁₉H₁₇N₅

SR CA

LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

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L2 ANSWER 9 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 541503-75-7 REGISTRY

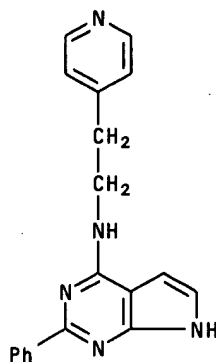
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FS 3D CONCORD

MF C₁₉H₁₇N₅

SR CA

LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

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STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE

14

L2 ANSWER 10 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 541503-73-5 REGISTRY

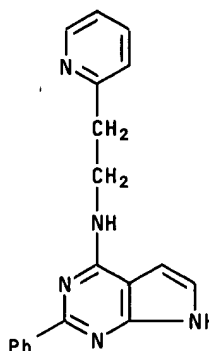
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FS 3D CONCORD

MF C₁₉H₁₇N₅

SR CA

LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

139:36534

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE

15

L2 ANSWER 11 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 541503-71-3 REGISTRY

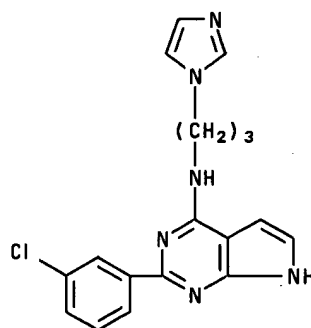
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 2-(3-chlorophenyl)-*N*-[3-(1*H*-imidazol-1-yl)propyl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₁₈H₁₇ClN₆

SR CA

LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

139:36534

L2 ANSWER 12 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 541503-69-9 REGISTRY

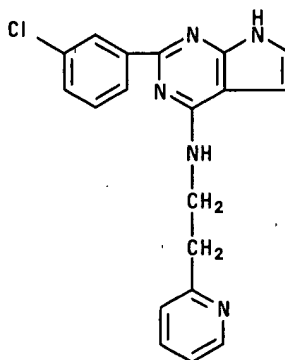
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 2-(3-chlorophenyl)-*N*-[2-(2-pyridinyl)ethyl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₁₉H₁₆ClN₅

SR CA

LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

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L2 ANSWER 13 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 541503-67-7 REGISTRY

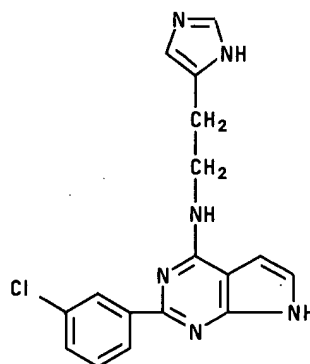
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 2-(3-chlorophenyl)-*N*-[2-(1*H*-imidazol-4-yl)ethyl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₁₇H₁₅ClN₆

SR CA

LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

139:36534

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

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18

L2 ANSWER 14 OF 249 REGISTRY COPYRIGHT 2004 ACS

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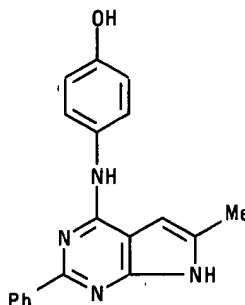
CN Phenol, 4-[(6-methyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

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SR CA

LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

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REFERENCE 1:

139:36534

L2 ANSWER 15 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 512848-48-5 REGISTRY

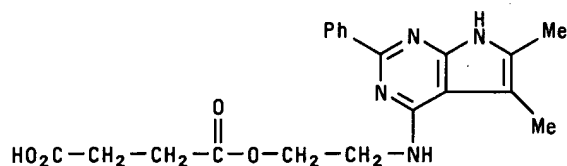
CN Butanedioic acid, mono[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl] ester
(9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₂₀H₂₂N₄O₄

SR CA

LC STN Files: CA, CAPLUS, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

138:321287

L2 ANSWER 16 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 512848-47-4 REGISTRY

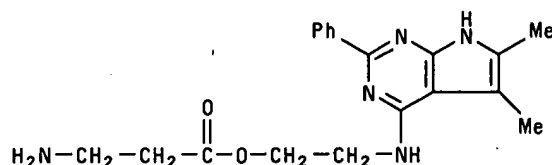
CN β -Alanine, 2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl ester (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₁₉H₂₃N₅O₂

SR CA

LC STN Files: CA, CAPLUS, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

138:321287

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

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L2 ANSWER 17 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 500736-10-7 REGISTRY

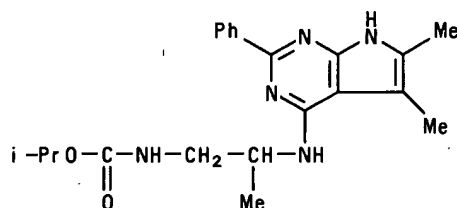
CN Carbamic acid, [2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]propyl]-, 1-methylethyl ester (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₂₁H₂₇N₅O₂

SR CA

LC STN Files: CA, CAPLUS, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

138:221598

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

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22

L2 ANSWER 18 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 500736-09-4 REGISTRY

CN Cyclohexanol,

4-[[2-(3-furanyl)-5,6-dimethyl-7-[(1*R*)-1-phenylethyl]-7*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl]amino]-, *trans*-
(9*CI*) (CA INDEX NAME)

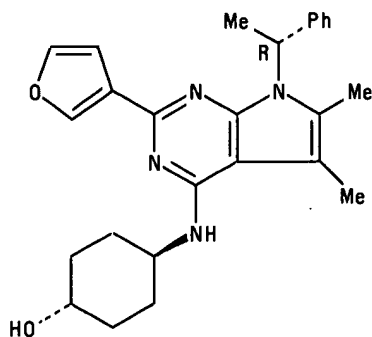
FS STEREOSEARCH

MF C₂₆H₃₀N₄O₂

SR CA

LC STN Files: CA, CAPLUS, USPAT2, USPATFULL

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

138:221598

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

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23

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RN 500736-03-8 REGISTRY

CN Glycine, (1*R*,3*S*)-3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]cyclopentyl ester, *rel*-, trifluoroacetate (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF $C_{21}H_{25}N_5O_2 \cdot xC_2HF_3O_2$

SR CA

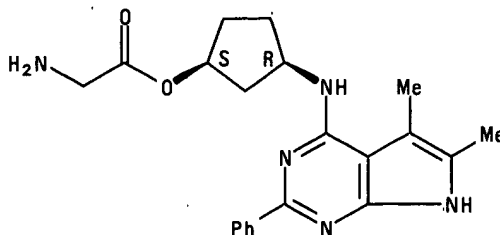
LC STN Files: CA, CAPLUS, USPAT2, USPATFULL

CM 1

CRN 251946-51-7

CMF $C_{21}H_{25}N_5O_2$

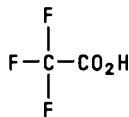
Relative stereochemistry.



CM 2

CRN 76-05-1

CMF $C_2HF_3O_2$



2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

138:321287

REFERENCE 2:

138:221598

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

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RN 500736-02-7 REGISTRY

CN Carbamic acid, [1-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]propyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

OTHER NAMES:

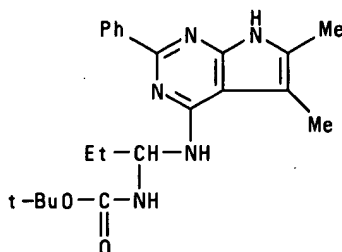
CN 4-[[2-Methyl-1-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS 3D CONCORD

MF C₂₂H₂₉N₅O₂

SR CA

LC STN Files: CA, CAPLUS, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

138:221598

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REGISTRY FILE SEARCH RESULTS - P077138C

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25

L2 ANSWER 21 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 476006-54-9 REGISTRY

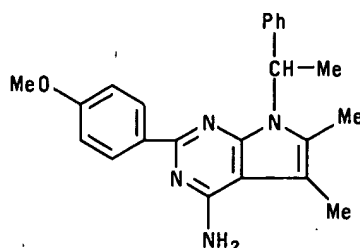
CN 7H-Pyrrolo[2,3-d]pyrimidin-4-amine, 2-(4-methoxyphenyl)-5,6-dimethyl-7-(1-phenylethyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₂₃H₂₄N₄O

SR CA

LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:379680

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RN 443760-85-8 REGISTRY

CN Methanesulfonamide,

N-[*trans*-4-[[5,6-dimethyl-2-phenyl-7-(1-phenylethyl)-7*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl]amino]cyclohexyl]- (9CI) (CA INDEX NAME)

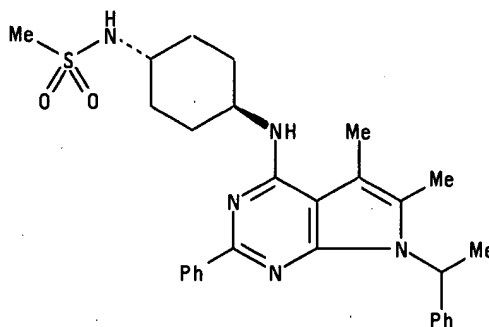
FS STEREOSEARCH

MF C₂₉H₃₅N₅O₂S

SR CA

LC STN Files: CA, CAPLUS, USPAT2, USPATFULL

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

138:221598

REFERENCE 2:

137:109485

L2 ANSWER 23 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443760-84-7 REGISTRY

CN Acetamide,

N-[*trans*-4-[[5,6-dimethyl-2-phenyl-7-(1-phenylethyl)-7*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl]amino]cyclohexyl]- (9CI) (CA INDEX NAME)

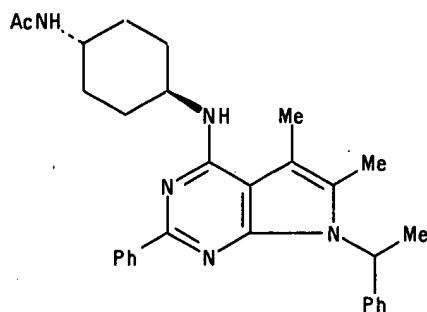
FS STEREOSEARCH

MF C₃₀H₃₅N₅O

SR CA

LC STN Files: CA, CAPLUS, USPAT2, USPATFULL

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

138:221598

REFERENCE 2:

137:109485

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L2 ANSWER 24 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443760-82-5 REGISTRY

CN Propanamide,

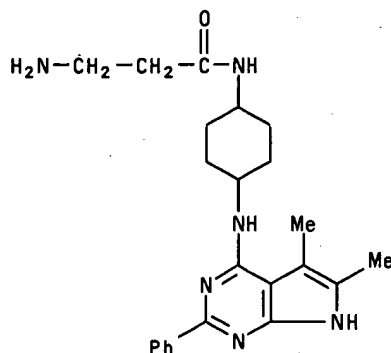
3-amino-N-[4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]cyclohexyl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₂₃H₃₀N₆O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

139:133575

REFERENCE 2:

138:221598

REFERENCE 3:

137:109485

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REGISTRY FILE SEARCH RESULTS - P077138C

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L2 ANSWER 25 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443760-80-3 REGISTRY

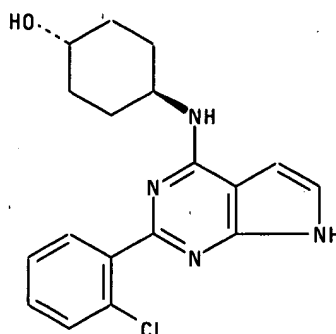
CN Cyclohexanol, 4-[[2-(2-chlorophenyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, *trans*- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C₁₈H₁₉ClN₄O

SR CA

LC STN Files: CA, CAPLUS
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109485

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RN 443760-79-0 REGISTRY

CN Cyclohexanol, 4-[[2-(2-fluorophenyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, *trans*- (9CI) (CA INDEX NAME)

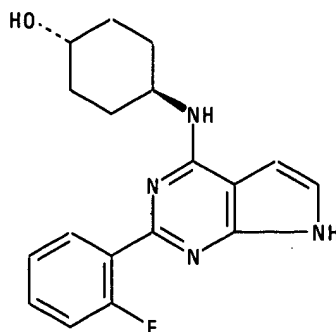
FS STEREOSEARCH

MF C₁₈H₁₉FN₄O

SR CA

LC STN Files: CA, CAPLUS

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109485

L2 ANSWER 27 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443760-78-9 REGISTRY

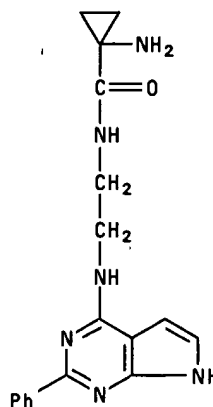
CN Cyclopropanecarboxamide, 1-amino-N-[2-[(2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]ethyl]- (9CI)
(CA INDEX NAME)

FS 3D CONCORD

MF C₁₈H₂₀N₆O

SR CA

LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109485

L2 ANSWER 28 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-78-3 REGISTRY

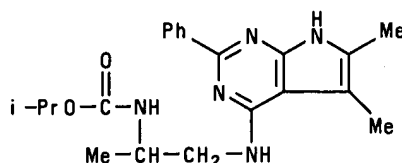
CN Carbamic acid, [2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-1-methylethyl]-, 1-methylethyl ester (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₂₁H₂₇N₅O₂

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

139:133575

REFERENCE 2:

138:221598

REFERENCE 3:

137:109288

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REGISTRY FILE SEARCH RESULTS - P077138C

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L2 ANSWER 29 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-73-8 REGISTRY

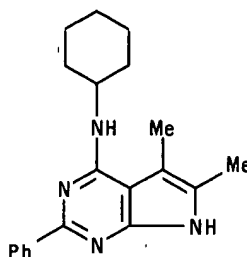
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, *N*-cyclohexyl-5,6-dimethyl-2-phenyl- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₂₀H₂₄N₄

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

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L2 ANSWER 30 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-72-7 REGISTRY

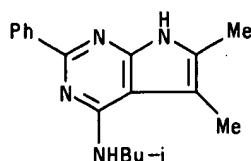
CN 1*H*-Pyrrolo[2,3-*d'*]pyrimidin-4-amine, 5,6-dimethyl-*N*-(2-methylpropyl)-2-phenyl- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₁₈H₂₂N₄

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

L2 ANSWER 31 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-71-6 REGISTRY

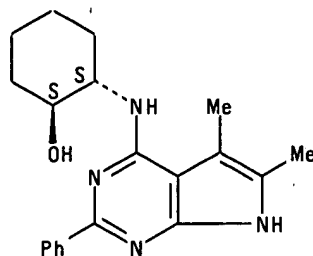
CN Cyclohexanol, 2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, (1*S*,2*S*)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C₂₀H₂₄N₄O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

L2 ANSWER 32 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-70-5 REGISTRY

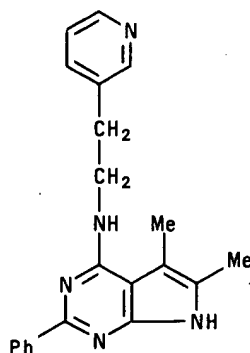
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 5,6-dimethyl-2-phenyl-*N*-[2-(3-pyridinyl)ethyl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₂₁H₂₁N₅

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



****PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT****

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

L2 ANSWER 33 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-69-2 REGISTRY

CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine,

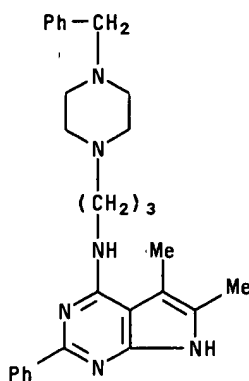
5,6-dimethyl-2-phenyl-*N*-[3-[4-(phenylmethyl)-1-piperazinyl]propyl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₂₈H₃₄N₆

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

L2 ANSWER 34 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-68-1 REGISTRY

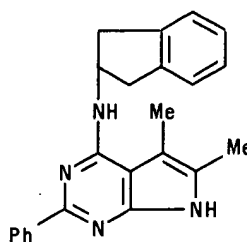
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, *N*-(2,3-dihydro-1*H*-inden-2-yl)-5,6-dimethyl-2-phenyl- (9CI)
(CA INDEX NAME)

FS 3D CONCORD

MF C₂₃H₂₂N₄

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

L2 ANSWER 35 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-67-0 REGISTRY

CN Benzenepropanol, 4-chloro- β -[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, (*βR*)-
(9CI) (CA INDEX NAME)

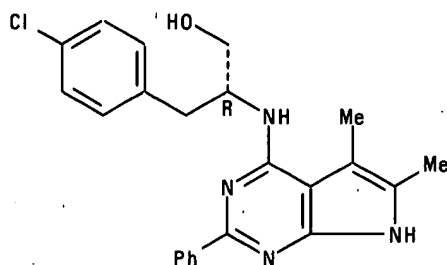
FS STEREOSEARCH

MF C₂₃H₂₃ClN₄O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

L2 ANSWER 36 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-66-9 REGISTRY

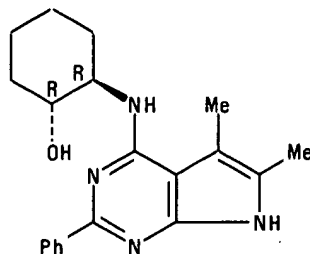
CN Cyclohexanol, 2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]-, (1*R*,2*R*)- (9CI)
(CA INDEX NAME)

FS STEREOSEARCH

MF C₂₀H₂₄N₄O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

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L2 ANSWER 37 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-65-8 REGISTRY

CN Benzenemethanol,

α -[(1S)-1-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-2-methoxyethyl]-, (αR)-
(9CI) (CA INDEX NAME)

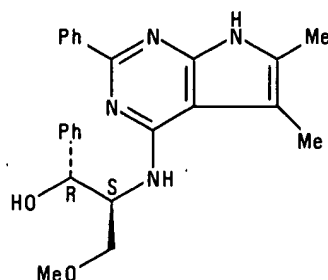
FS STEREOSEARCH

MF C₂₄H₂₆N₄O₂

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

L2 ANSWER 38 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-64-7 REGISTRY

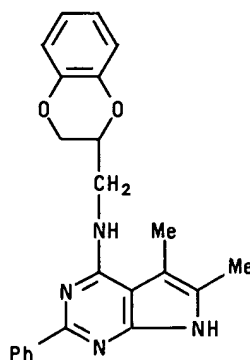
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine,*N*-[(2,3-dihydro-1,4-benzodioxin-2-yl)methyl]-5,6-dimethyl-2-phenyl- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₂₃H₂₂N₄O₂

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

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REGISTRY FILE SEARCH RESULTS - P077138C

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L2 ANSWER 39 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-63-6 REGISTRY

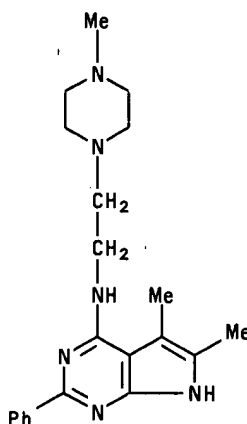
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 5,6-dimethyl-*N*-[2-(4-methyl-1-piperazinyl)ethyl]-2-phenyl- (9CI)
(CA INDEX NAME)

FS 3D CONCORD

MF C₂₁H₂₈N₆

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

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REGISTRY FILE SEARCH RESULTS - P077138C

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L2 ANSWER 40 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-62-5 REGISTRY

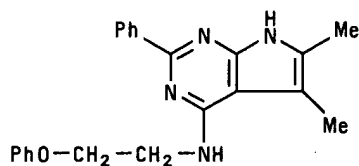
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 5,6-dimethyl-*N*-(2-phenoxyethyl)-2-phenyl- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₂₂H₂₂N₄O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

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REGISTRY FILE SEARCH RESULTS - P077138C

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L2 ANSWER 41 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-61-4 REGISTRY

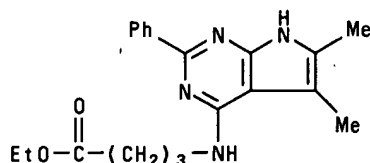
CN Butanoic acid, 4-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]-, ethyl ester (9CI)
(CA INDEX NAME)

FS 3D CONCORD

MF C₂₀H₂₄N₄O₂

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

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REGISTRY FILE SEARCH RESULTS - P077138C

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L2 ANSWER 42 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-60-3 REGISTRY

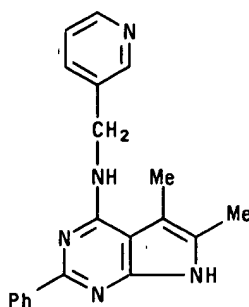
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 5,6-dimethyl-2-phenyl-*N*-(3-pyridinylmethyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₂₀H₁₉N₅

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



****PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT****

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

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REGISTRY FILE SEARCH RESULTS - P077138C

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47

L2 ANSWER 43 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-59-0 REGISTRY

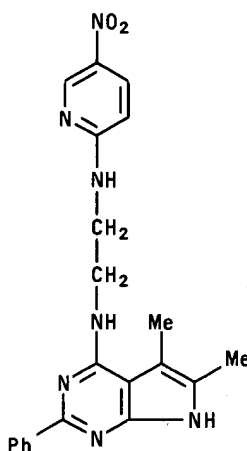
CN 1,2-Ethanediamine, *N*-(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)-*N'*-(5-nitro-2-pyridinyl)-
(9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₂₁H₂₁N₇O₂

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



****PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT****

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

L2 ANSWER 44 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-58-9 REGISTRY

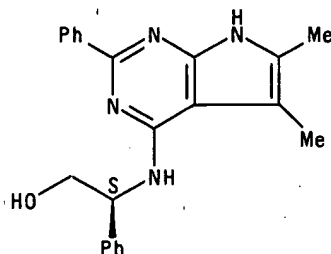
CN Benzeneethanol, β -[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]-, (β S)- (9CI)
(CA INDEX NAME)

FS STEREOSEARCH

MF C₂₂H₂₂N₄O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

L2 ANSWER 45 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-57-8 REGISTRY

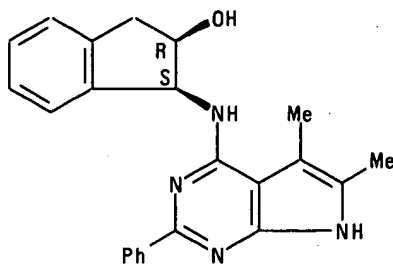
CN 1*H*-Inden-2-ol, 1-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]-2,3-dihydro-,
(1*S*,2*R*)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C₂₃H₂₂N₄O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

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L2 ANSWER 46 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-56-7 REGISTRY

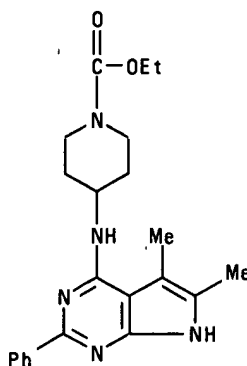
CN 1-Piperidinecarboxylic acid, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, ethyl ester (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₂₂H₂₇N₅O₂

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

L2 ANSWER 47 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-55-6 REGISTRY

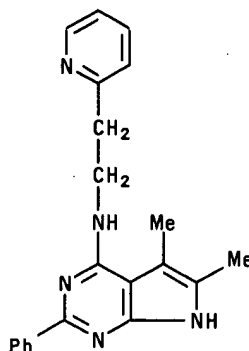
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 5,6-dimethyl-2-phenyl-*N*-[2-(2-pyridinyl)ethyl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₂₁H₂₁N₅

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

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REGISTRY FILE SEARCH RESULTS - P077138C

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52

L2 ANSWER 48 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-54-5 REGISTRY

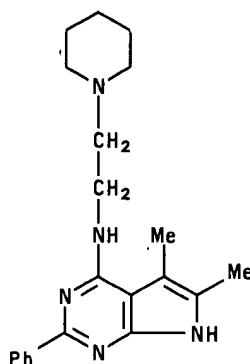
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 5,6-dimethyl-2-phenyl-*N*-[2-(1-piperidinyl)ethyl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₂₁H₂₇N₅

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

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L2 ANSWER 49 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-53-4 REGISTRY

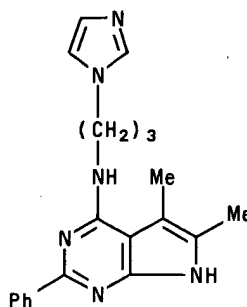
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, *N*-[3-(1*H*-imidazol-1-yl)propyl]-5,6-dimethyl-2-phenyl- (9CI)
(CA INDEX NAME)

FS 3D CONCORD

MF C₂₀H₂₂N₆

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

L2 ANSWER 50 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-52-3 REGISTRY

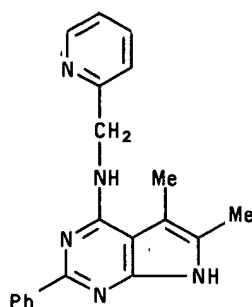
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 5,6-dimethyl-2-phenyl-*N*-(2-pyridinylmethyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₂₀H₁₉N₅

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

L2 ANSWER 51 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-51-2 REGISTRY

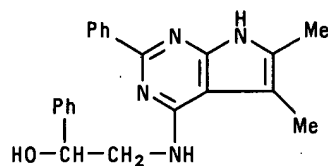
CN Benzenemethanol, α -[[[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]methyl]- (9CI)
(CA INDEX NAME)

FS 3D CONCORD

MF C₂₂H₂₂N₄O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

L2 ANSWER 52 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-50-1 REGISTRY

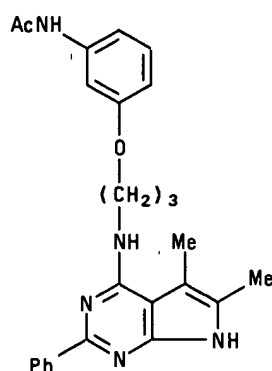
CN Acetamide, *N*-[3-[3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]propoxy]phenyl]-
(9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₂₅H₂₇N₅O₂

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

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L2 ANSWER 53 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-49-8 REGISTRY

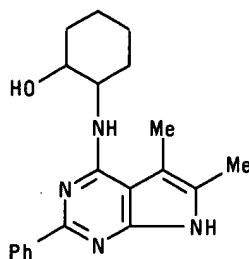
CN Cyclohexanol, 2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₂₀H₂₄N₄O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

L2 ANSWER 54 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-48-7 REGISTRY

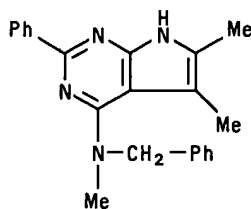
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, *N*,5,6-trimethyl-2-phenyl-*N*-(phenylmethyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₂₂H₂₂N₄

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

L2 ANSWER 55 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-47-6 REGISTRY

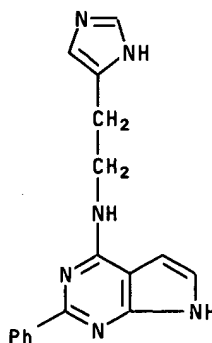
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, *N*-[2-(1*H*-imidazol-4-yl)ethyl]-2-phenyl- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₁₇H₁₆N₆

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1907 TO DATE)

4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

139:36534

REFERENCE 2:

138:321287

REFERENCE 3:

137:109485

REFERENCE 4:

137:109288

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L2 ANSWER 56 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-46-5 REGISTRY

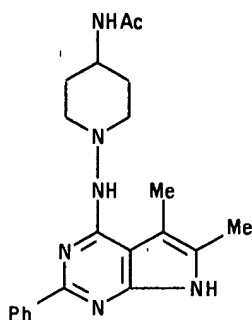
CN Acetamide, *N*-[1-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-4-piperidiny]- (9CI)
(CA INDEX NAME)

FS 3D CONCORD

MF C₂₁H₂₆N₆O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

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L2 ANSWER 57 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-45-4 REGISTRY

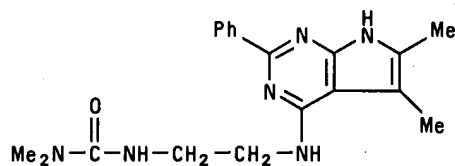
CN Urea, *N'*-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]-*N,N*-dimethyl-
(9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₁₉H₂₄N₆O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

L2 ANSWER 58 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-44-3 REGISTRY

CN Cyclohexanol,

4-[[5,6-dimethyl-2-phenyl-7-[(1S)-1-phenylethyl]-7H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, *trans*-
(9CI) (CA INDEX NAME)

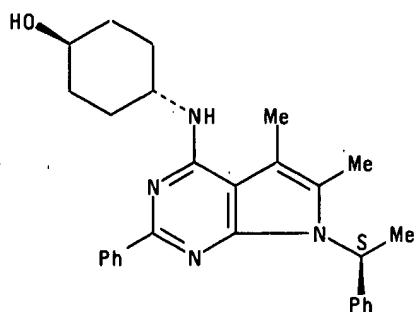
FS STEREOSEARCH

MF C₂₈H₃₂N₄O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

139:133575

REFERENCE 2:

137:109288

L2 ANSWER 59 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-43-2 REGISTRY

CN Cyclohexanol,

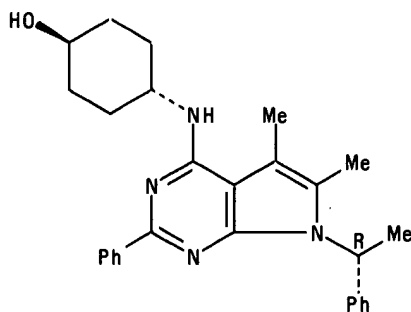
4-[[5,6-dimethyl-2-phenyl-7-[(1*R*)-1-phenylethyl]-7*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl]amino]-, *trans*-
(9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C₂₈H₃₂N₄O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

139:133575

REFERENCE 2:

138:221598

REFERENCE 3:

137:109288

L2 ANSWER 60 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-42-1 REGISTRY

CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 5,6-dimethyl-*N*-(*trans*-4-methylcyclohexyl)-2-phenyl- (9CI)
(CA INDEX NAME)

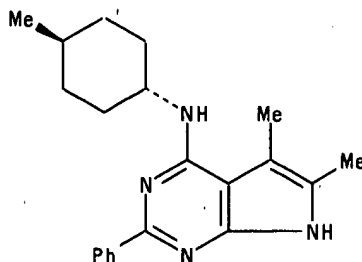
FS STEREOSEARCH

MF C₂₁H₂₆N₄

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

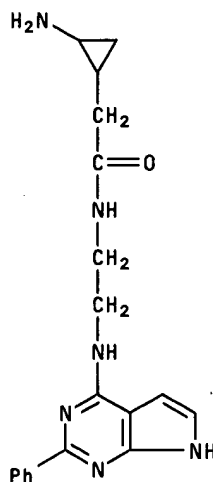
1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

L2 ANSWER 61 OF 249 REGISTRY COPYRIGHT 2004 ACS
RN 443118-41-0 REGISTRY
CN Cyclopropaneacetamide, 2-amino-*N*-[2-[(2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]ethyl]- (9CI)
(CA INDEX NAME)
FS 3D CONCORD
MF C₁₉H₂₂N₆O
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

L2 ANSWER 62 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-36-3 REGISTRY

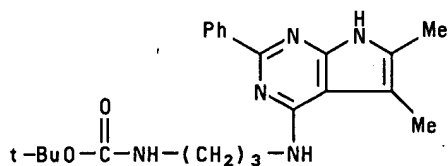
CN Carbamic acid, [3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]propyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₂₂H₂₉N₅O₂

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

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L2 ANSWER 63 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-26-1 REGISTRY

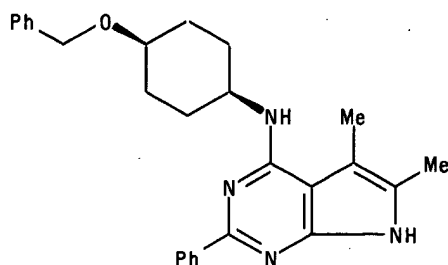
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 5,6-dimethyl-2-phenyl-*N*-[*cis*-4-(phenylmethoxy)cyclohexyl]-
(9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C₂₇H₃₀N₄O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

L2 ANSWER 64 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-24-9 REGISTRY

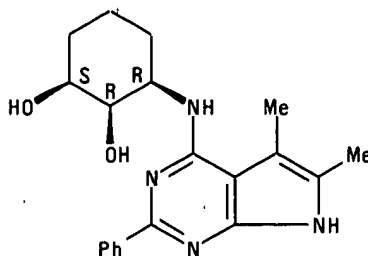
CN 1,2-Cyclohexanediol, 3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]-, (1*R*,2*S*,3*S*)-*rel*- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C₂₀H₂₄N₄O₂

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

L2 ANSWER 65 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-23-8 REGISTRY

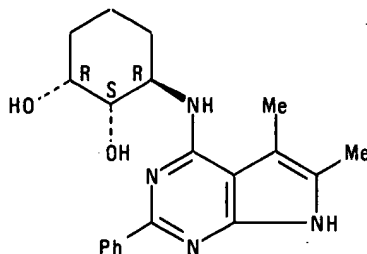
CN 1,2-Cyclohexanediol, 3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]-,
(1*R*,2*S*,3*R*)-*rel*- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C₂₀H₂₄N₄O₂

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

L2 ANSWER 66 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 443118-22-7 REGISTRY

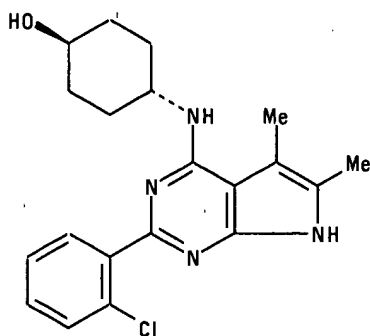
CN Cyclohexanol, 4-[[2-(2-chlorophenyl)-5,6-dimethyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl]amino]-, *trans*-
(9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C₂₀H₂₃ClN₄O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

L2 ANSWER 67 OF 249 REGISTRY COPYRIGHT 2004 ACS

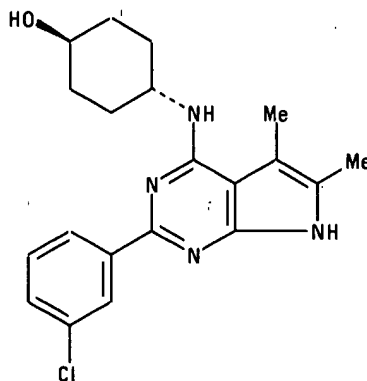
RN 443118-21-6 REGISTRY

CN Cyclohexanol, 4-[[2-(3-chlorophenyl)-5,6-dimethyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl]amino]-, *trans*-
(9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C₂₀H₂₃ClN₄O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL
Relative stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

L2 ANSWER 68 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 412342-10-0 REGISTRY

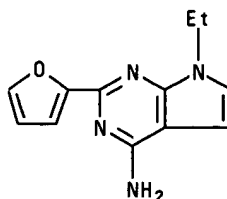
CN 7H-Pyrrolo[2,3-d']pyrimidin-4-amine, 7-ethyl-2-(2-furanyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₁₂H₁₂N₄O

SR Reaction Database

LC STN Files: CASREACT



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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RN 343969-97-1 REGISTRY

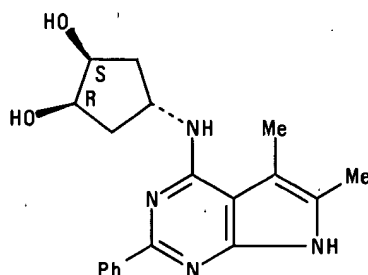
CN 1,2-Cyclopentanediol, 4-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]-, (1*α*,2*α*,4*β*)-(9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C₁₉H₂₂N₄O₂

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

7 REFERENCES IN FILE CA (1907 TO DATE)

7 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:221598

REFERENCE 4:

137:109485

REFERENCE 5:

137:109288

REFERENCE 6:

136:386128

REFERENCE 7:

135:46190

L2 ANSWER 70 OF 249 REGISTRY COPYRIGHT 2004 ACS

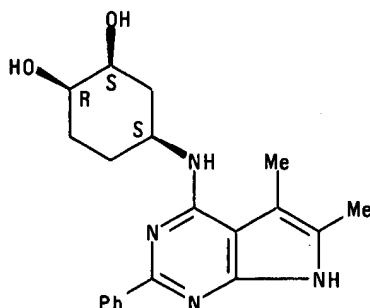
RN 343969-79-9 REGISTRY

CN 1,2-Cyclohexanediol, 4-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-,
(1*R*,2*S*,4*S*)-*rel*- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C₂₀H₂₄N₄O₂

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL
Relative stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

6 REFERENCES IN FILE CA (1907 TO DATE)

6 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:221598

REFERENCE 4:

137:109485

REFERENCE 5:

136:386128

REFERENCE 6:

135:46190

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RN 343633-16-9 REGISTRY

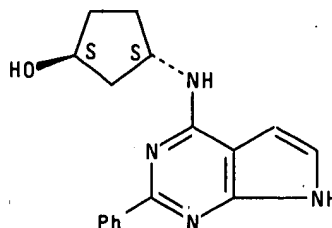
CN Cyclopentanol, 3-[(2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, (1*S*,3*S*)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C₁₇H₁₈N₄O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1907 TO DATE)

4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

137:109288

REFERENCE 3:

136:386128

REFERENCE 4:

135:46190

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REGISTRY FILE SEARCH RESULTS - P077138C

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L2 ANSWER 72 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-97-3 REGISTRY

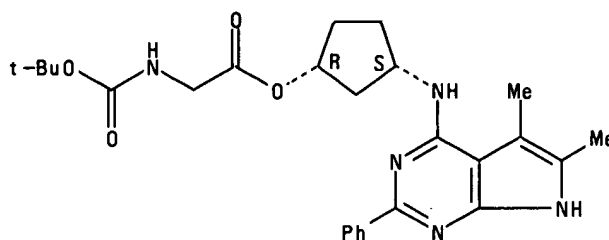
CN Glycine, *N*-[(1,1-dimethylethoxy)carbonyl]-,
(1*R*,3*S*)-3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]cyclopentyl ester, *rel*- (9CI)
(CA INDEX NAME)

FS STEREOSEARCH

MF C₂₆H₃₃N₅O₄

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

5 REFERENCES IN FILE CA (1907 TO DATE)

5 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

138:221598

REFERENCE 3:

137:109288

REFERENCE 4:

136:386128

REFERENCE 5:

135:46190

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REGISTRY FILE SEARCH RESULTS - P077138C

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L2 ANSWER 73 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-96-2 REGISTRY

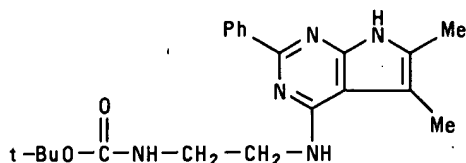
CN Carbamic acid, [2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₂₁H₂₇N₅O₂

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



****PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT****

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

136:386128

REFERENCE 3:

135:46190

L2 ANSWER 74 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-79-1 REGISTRY

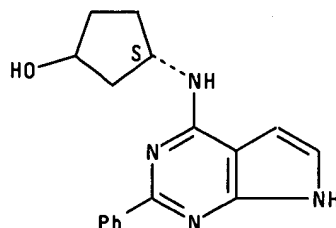
CN Cyclopentanol, 3-[(2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, (3*S*)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C₁₇H₁₈N₄O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1907 TO DATE)

4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

137:109288

REFERENCE 3:

136:386128

REFERENCE 4:

135:46190

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REGISTRY FILE SEARCH RESULTS - P077138C

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L2 ANSWER 75 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-78-0 REGISTRY

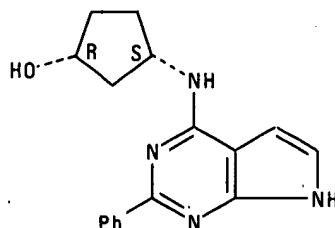
CN Cyclopentanol, 3-[(2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, (1*R*,3*S*)- (CA INDEX NAME)

FS STEREOSEARCH

MF C₁₇H₁₈N₄O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1907 TO DATE)

4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

137:109288

REFERENCE 3:

136:386128

REFERENCE 4:

135:46190

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RN 343632-77-9 REGISTRY

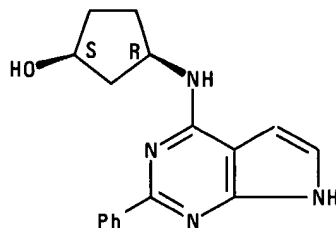
CN Cyclopentanol, 3-[(2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, (1*S*,3*R*)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C₁₇H₁₈N₄O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1907 TO DATE)

4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

137:109288

REFERENCE 3:

136:386128

REFERENCE 4:

135:46190

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RN 343632-73-5 REGISTRY

CN Urea,

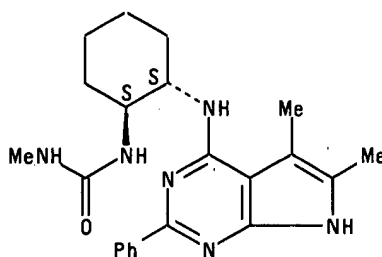
N-[(1*S*,2*S*)-2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]cyclohexyl]-*N'*-methyl-
(9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C₂₂H₂₈N₆O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

136:386128

REFERENCE 3:

135:46190

L2 ANSWER 78 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-72-4 REGISTRY

CN Urea,

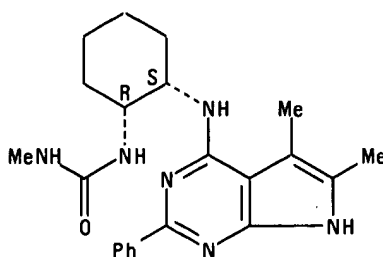
N-[(1*R*,2*S*)-2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]cyclohexyl]-*N'*-methyl-
(9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C₂₂H₂₈N₆O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

136:386128

REFERENCE 3:

135:46190

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RN 343632-71-3 REGISTRY

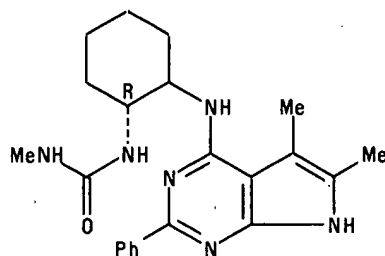
CN Urea, *N*-[(1*R*)-2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]cyclohexyl]-*N'*-methyl-
(9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C₂₂H₂₈N₆O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL
Absolute stereochemistry.



****PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT****

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

136:386128

REFERENCE 3:

135:46190

L2 ANSWER 80 OF 249 REGISTRY COPYRIGHT 2004 ACS

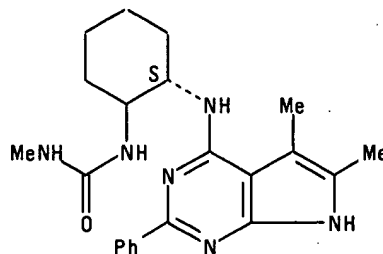
RN 343632-70-2 REGISTRY

CN Urea, *N*-[(2*S*)-2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]cyclohexyl]-*N'*-methyl-
(9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C₂₂H₂₈N₆O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL
Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

136:386128

REFERENCE 3:

135:46190

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L2 ANSWER 81 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-69-9 REGISTRY

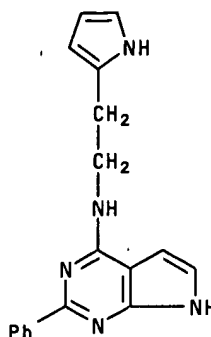
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 2-phenyl-*N*-[2-(1*H*-pyrrol-2-yl)ethyl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₁₈H₁₇N₅

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



***PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

136:386128

REFERENCE 2:

135:46190

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L2 ANSWER 82 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-50-8 REGISTRY

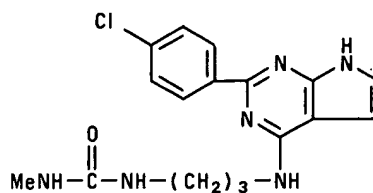
CN Urea, *N*-[3-[[2-(4-chlorophenyl)-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl]amino]propyl]-*N'*-methyl- (9CI)
(CA INDEX NAME)

FS 3D CONCORD

MF C₁₇H₁₉ClN₆O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

7 REFERENCES IN FILE CA (1907 TO DATE)

7 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

139:36534

REFERENCE 4:

138:321287

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

135:46190

L2 ANSWER 83 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-38-2 REGISTRY

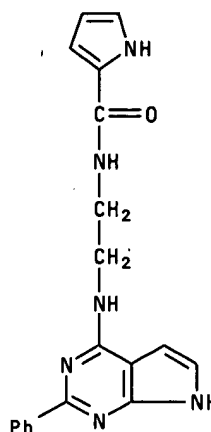
CN 1*H*-Pyrrole-2-carboxamide, *N*-[2-[(2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₁₉H₁₈N₆O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

7 REFERENCES IN FILE CA (1907 TO DATE)

7 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

139:36534

REFERENCE 4:

138:321287

REFERENCE 5:

137:109485

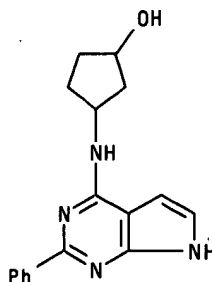
REFERENCE 6:

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L2 ANSWER 83 OF 249 REGISTRY COPYRIGHT 2004 ACS
RN 343632-38-2 REGISTRY
137:109288

REFERENCE 7:
135:46190

L2 ANSWER 84 OF 249 REGISTRY COPYRIGHT 2004 ACS
RN 343632-37-1 REGISTRY
CN Cyclopentanol, 3-[(2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C₁₇H₁₈N₄O
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

7 REFERENCES IN FILE CA (1907 TO DATE)
7 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:
140:146159

REFERENCE 2:
139:133575

REFERENCE 3:
139:36534

REFERENCE 4:
138:321287

REFERENCE 5:

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RN 343632-37-1 REGISTRY

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

135:46190

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RN 343632-36-0 REGISTRY

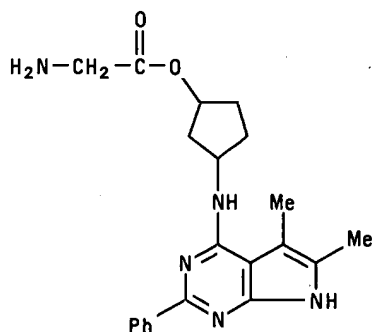
CN Glycine, 3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]cyclopentyl ester (9CI)
(CA INDEX NAME)

FS 3D CONCORD

MF C₂₁H₂₅N₅O₂

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

5 REFERENCES IN FILE CA (1907 TO DATE)

5 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

139:36534

REFERENCE 4:

137:109288

REFERENCE 5:

135:46190

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L2 ANSWER 86 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-35-9 REGISTRY

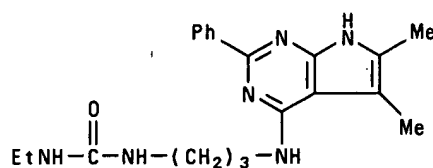
CN Urea, *N*-[3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]propyl]-*N'*-ethyl- (9CI)
(CA INDEX NAME)

FS 3D CONCORD

MF C₂₀H₂₆N₆O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

7 REFERENCES IN FILE CA (1907 TO DATE)

7 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

139:36534

REFERENCE 4:

138:321287

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

135:46190

L2 ANSWER 87 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-33-7 REGISTRY

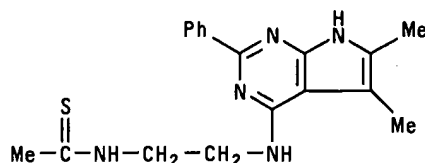
CN Ethanethioamide, *N*-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]- (9CI)
(CA INDEX NAME)

FS 3D CONCORD

MF C₁₈H₂₁N₅S

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

5 REFERENCES IN FILE CA (1907 TO DATE)

5 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

139:36534

REFERENCE 4:

137:109288

REFERENCE 5:

135:46190

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RN 343632-32-6 REGISTRY

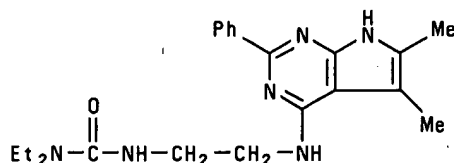
CN Urea, *N'*-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]ethyl]-*N,N*-diethyl- (9CI)
(CA INDEX NAME)

FS 3D CONCORD

MF C₂₁H₂₈N₆O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

6 REFERENCES IN FILE CA (1907 TO DATE)

6 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

139:36534

REFERENCE 4:

138:321287

REFERENCE 5:

137:109288

REFERENCE 6:

135:46190

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RN 343632-31-5 REGISTRY

CN Acetamide,

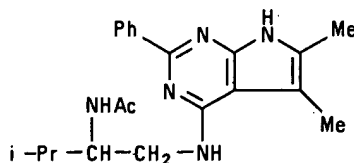
N-[1-[[[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]methyl]-2-methylpropyl]- (9CI)
(CA INDEX NAME)

FS 3D CONCORD

MF C₂₁H₂₇N₅O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

7 REFERENCES IN FILE CA (1907 TO DATE)

7 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

139:36534

REFERENCE 4:

138:321287

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

135:46190

L2 ANSWER 90 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-21-3 REGISTRY

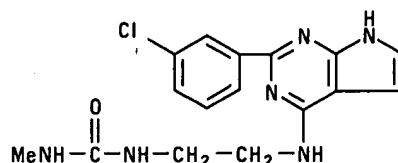
CN Urea, *N*-[2-[[2-(3-chlorophenyl)-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl]amino]ethyl]-*N'*-methyl- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₁₆H₁₇ClN₆O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

5 REFERENCES IN FILE CA (1907 TO DATE)

5 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

139:133575

REFERENCE 2:

138:221598

REFERENCE 3:

137:109485

REFERENCE 4:

136:386128

REFERENCE 5:

135:46190

L2 ANSWER 91 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-20-2 REGISTRY

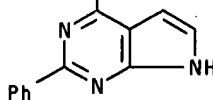
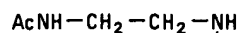
CN Acetamide, *N*-[2-[(2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₁₆H₁₇N₅O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

5 REFERENCES IN FILE CA (1907 TO DATE)

5 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

139:133575

REFERENCE 2:

138:221598

REFERENCE 3:

137:109485

REFERENCE 4:

136:386128

REFERENCE 5:

135:46190

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REGISTRY FILE SEARCH RESULTS - P077138C

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RN 343632-19-9 REGISTRY

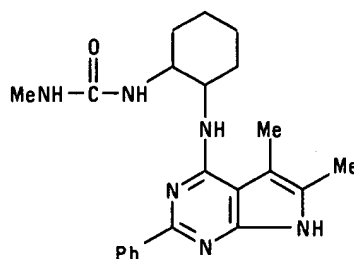
CN Urea, *N*-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]cyclohexyl]-*N'*-methyl-
(9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₂₂H₂₈N₆O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

5 REFERENCES IN FILE CA (1907 TO DATE)

5 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

139:133575

REFERENCE 2:

138:221598

REFERENCE 3:

137:109485

REFERENCE 4:

136:386128

REFERENCE 5:

135:46190

L2 ANSWER 93 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-17-7 REGISTRY

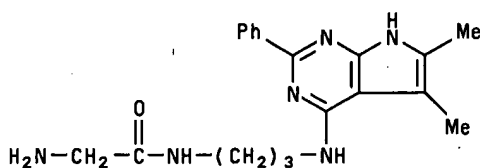
CN Acetamide, 2-amino-*N*-[3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]propyl]-
(9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₁₉H₂₄N₆O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



****PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT****

7 REFERENCES IN FILE CA (1907 TO DATE)

7 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

139:133575

REFERENCE 2:

138:321287

REFERENCE 3:

138:221598

REFERENCE 4:

137:109485

REFERENCE 5:

137:109288

REFERENCE 6:

136:386128

REFERENCE 7:

135:46190

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RN 343632-16-6 REGISTRY

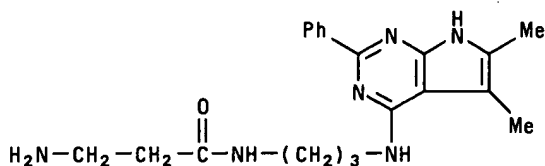
CN Propanamide, 3-amino-*N*-[3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]propyl]-
(9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₂₀H₂₆N₆O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

5 REFERENCES IN FILE CA (1907 TO DATE)

5 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

139:133575

REFERENCE 2:

138:221598

REFERENCE 3:

137:109485

REFERENCE 4:

136:386128

REFERENCE 5:

135:46190

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REGISTRY FILE SEARCH RESULTS - P077138C

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L2 ANSWER 95 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-15-5 REGISTRY

CN Cyclopropanecarboxamide,

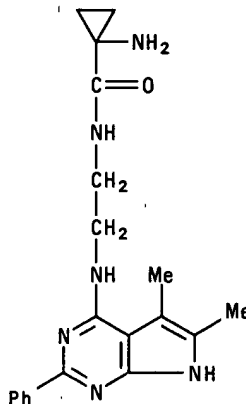
1-amino-N-[2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]ethyl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₂₀H₂₄N₆O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

6 REFERENCES IN FILE CA (1907 TO DATE)

6 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:221598

REFERENCE 4:

137:109288

REFERENCE 5:

136:386128

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REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 101

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RN 343632-15-5 REGISTRY

REFERENCE 6:

135:46190

L2 ANSWER 96 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-14-4 REGISTRY

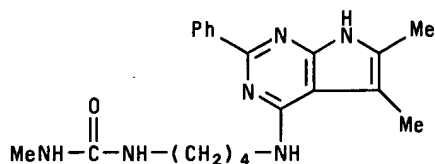
CN Urea, *N*-[4-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]butyl]-*N'*-methyl- (9CI)
(CA INDEX NAME)

FS 3D CONCORD

MF C₂₀H₂₆N₆O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

7 REFERENCES IN FILE CA (1907 TO DATE)

7 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:221598

REFERENCE 4:

137:109485

REFERENCE 5:

137:109288

REFERENCE 6:

136:386128

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REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 102
L2 ANSWER 96 OF 249 REGISTRY COPYRIGHT 2004 ACS
RN 343632-14-4 REGISTRY

REFERENCE 7:

135:46190

L2 ANSWER 97 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-13-3 REGISTRY

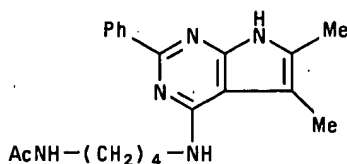
CN Acetamide, *N*-[4-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]butyl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₂₀H₂₅N₅O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

7 REFERENCES IN FILE CA (1907 TO DATE)

7 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:221598

REFERENCE 4:

137:109485

REFERENCE 5:

137:109288

REFERENCE 6:

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L2 ANSWER 97 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-13-3 REGISTRY

136:386128

REFERENCE 7:

135:46190

L2 ANSWER 98 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-12-2 REGISTRY

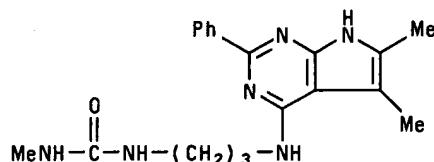
CN Urea, *N*-[3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]propyl]-*N'*-methyl- (9CI)
(CA INDEX NAME)

FS 3D CONCORD

MF C₁₉H₂₄N₆O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

6 REFERENCES IN FILE CA (1907 TO DATE)

6 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:221598

REFERENCE 4:

137:109485

REFERENCE 5:

136:386128

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RN 343632-12-2 REGISTRY

REFERENCE 6:

135:46190

L2 ANSWER 99 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-11-1 REGISTRY

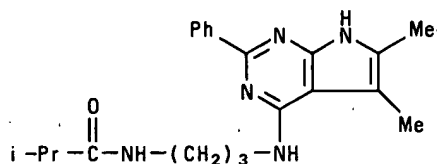
CN Propanamide, *N*-[3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]propyl]-2-methyl-
(9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₂₁H₂₇N₅O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

7 REFERENCES IN FILE CA (1907 TO DATE)

7 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:221598

REFERENCE 4:

137:109485

REFERENCE 5:

137:109288

REFERENCE 6:

136:386128

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REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 105
L2 ANSWER 99 OF 249 REGISTRY COPYRIGHT 2004 ACS
RN 343632-11-1 REGISTRY

REFERENCE 7:

135:46190

L2 ANSWER 100 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-10-0 REGISTRY

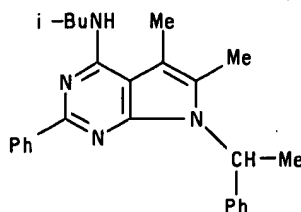
CN 7*H*-Pyrrolo[2,3-*d'*]pyrimidin-4-amine, 5,6-dimethyl-*N*-(2-methylpropyl)-2-phenyl-7-(1-phenylethyl)-
(9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₂₆H₃₀N₄

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

6 REFERENCES IN FILE CA (1907 TO DATE)

6 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:221598

REFERENCE 4:

137:109485

REFERENCE 5:

136:386128

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REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 106

L2 ANSWER 100 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-10-0 REGISTRY

REFERENCE 6:

135:46190

L2 ANSWER 101 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-09-7 REGISTRY

CN Acetamide,

N-[2-[[5,6-dimethyl-2-phenyl-7-(1-phenylethyl)-7*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl]amino]ethyl]- (9CI)

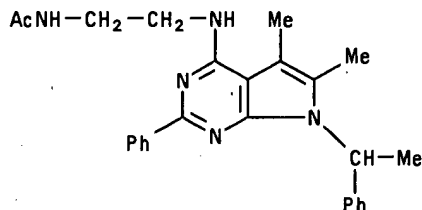
(CA INDEX NAME)

FS 3D CONCORD

MF C₂₆H₂₉N₅O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

6 REFERENCES IN FILE CA (1907 TO DATE)

6 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:221598

REFERENCE 4:

137:109485

REFERENCE 5:

136:386128

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 107

L2 ANSWER 101 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-09-7 REGISTRY

REFERENCE 6:

135:46190

L2 ANSWER 102 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-08-6 REGISTRY

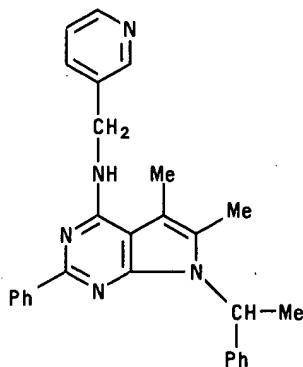
CN 7*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 5,6-dimethyl-2-phenyl-7-(1-phenylethyl)-*N*-(3-pyridinylmethyl)-
(9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₂₈H₂₇N₅

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

6 REFERENCES IN FILE CA (1907 TO DATE)

6 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:221598

REFERENCE 4:

137:109485

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 108
L2 ANSWER 102 OF 249 REGISTRY COPYRIGHT 2004 ACS
RN 343632-08-6 REGISTRY

REFERENCE 5:

136:386128

REFERENCE 6:

135:46190

L2 ANSWER 103 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-07-5 REGISTRY

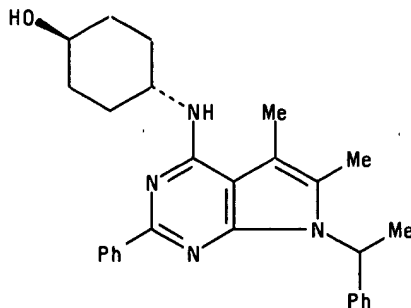
CN Cyclohexanol, 4-[[5,6-dimethyl-2-phenyl-7-(1-phenylethyl)-7H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, *trans*- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C₂₈H₃₂N₄O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

6 REFERENCES IN FILE CA (1907 TO DATE)

6 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:221598

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REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 109

L2 ANSWER 103 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-07-5 REGISTRY

REFERENCE 4:

137:109485

REFERENCE 5:

136:386128

REFERENCE 6:

135:46190

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REGISTRY FILE SEARCH RESULTS - P077138C

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L2 ANSWER 104 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343632-06-4 REGISTRY

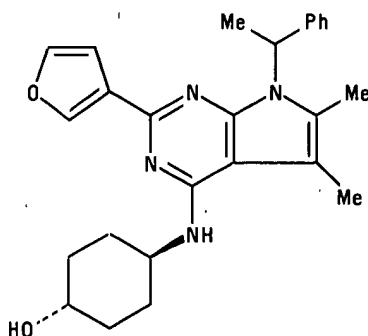
CN Cyclohexanol, 4-[[2-(3-furanyl)-5,6-dimethyl-7-(1-phenylethyl)-7H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, *trans*- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF $C_{26}H_{30}N_4O_2$

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL
Relative stereochemistry.



****PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT****

6 REFERENCES IN FILE CA (1907 TO DATE)

6 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

137:109485

REFERENCE 4:

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REFERENCE 5:

136:386128

REFERENCE 6:

135:46190

L2 ANSWER 105 OF 249 REGISTRY COPYRIGHT 2004 ACS

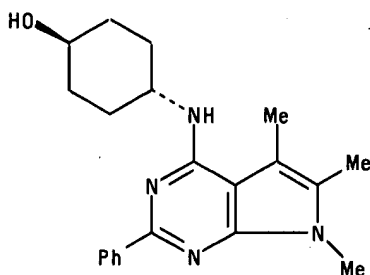
RN 343632-05-3 REGISTRY

CN Cyclohexanol, 4-[(5,6,7-trimethyl-2-phenyl-7H-pyrrolo[2,3-d']pyrimidin-4-yl)amino]-, *trans*- (9CI)
(CA INDEX NAME)

FS STEREOSEARCH

MF C₂₁H₂₆N₄O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL
Relative stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

6 REFERENCES IN FILE CA (1907 TO DATE)

6 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:221598

REFERENCE 4:

137:109485

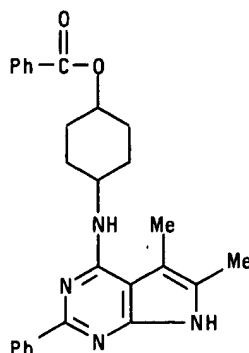
REFERENCE 5:

136:386128

REFERENCE 6:

135:46190

L2 ANSWER 106 OF 249 REGISTRY COPYRIGHT 2004 ACS
RN 343632-04-2 REGISTRY
CN Cyclohexanol, 4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, benzoate (ester)
(9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C₂₇H₂₈N₄O₂
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



***PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

6 REFERENCES IN FILE CA (1907 TO DATE)

6 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:221598

REFERENCE 4:

137:109288

REFERENCE 5:

136:386128

REFERENCE 6:

135:46190

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REGISTRY FILE SEARCH RESULTS - P077138C

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RN 343632-03-1 REGISTRY

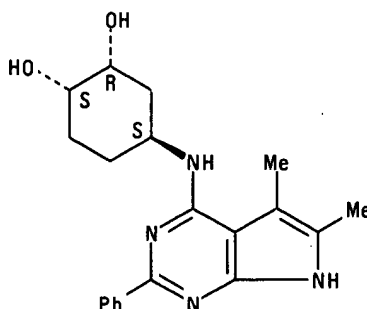
CN 1,2-Cyclohexanediol, 4-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, (1*R*,2*S*,4*R*)-*rel*- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C₂₀H₂₄N₄O₂

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

6 REFERENCES IN FILE CA (1907 TO DATE)

6 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:221598

REFERENCE 4:

137:109485

REFERENCE 5:

136:386128

REFERENCE 6:

135:46190

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REGISTRY FILE SEARCH RESULTS - P077138C

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L2 ANSWER 108 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343631-99-2 REGISTRY

CN Acetamide,

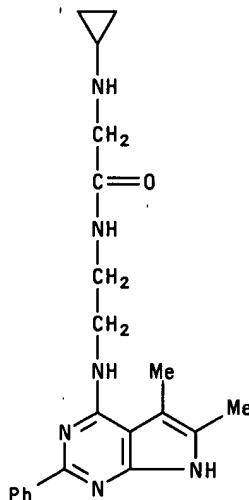
2-(cyclopropylamino)-*N*-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]- (9CI)
(CA INDEX NAME)

FS 3D CONCORD

MF C₂₁H₂₆N₆O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

136:386128

REFERENCE 3:

135:46190

L2 ANSWER 109 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343631-97-0 REGISTRY

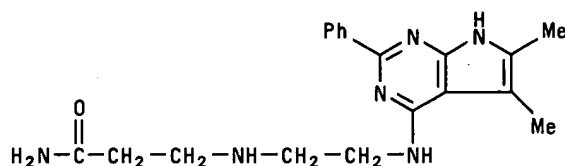
CN Propanamide, 3-[[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]amino]- (9CI)
(CA INDEX NAME)

FS 3D CONCORD

MF C₁₉H₂₄N₆O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

136:386128

REFERENCE 3:

135:46190

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

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L2 ANSWER 110 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343631-96-9 REGISTRY

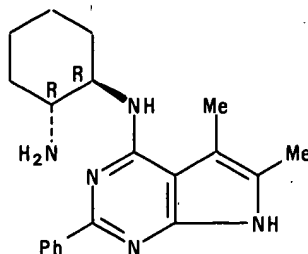
CN 1,2-Cyclohexanediamine, *N*-(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)-, (1*R*,2*R*)- (9CI)
(CA INDEX NAME)

FS STEREOSEARCH

MF C₂₀H₂₅N₅

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1907 TO DATE)

4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

138:321287

REFERENCE 3:

136:386128

REFERENCE 4:

135:46190

L2 ANSWER 111 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 343631-95-8 REGISTRY

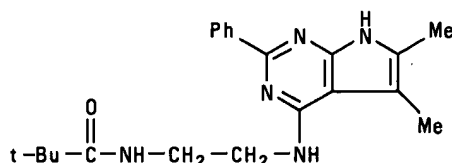
CN Propanamide, *N*-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]-2,2-dimethyl-
(9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₂₁H₂₇N₅O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

136:386128

REFERENCE 3:

135:46190

L2 ANSWER 112 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 341964-52-1 REGISTRY

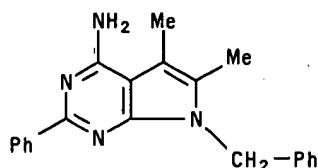
CN 7H-Pyrrolo[2,3-d]pyrimidin-4-amine, 5,6-dimethyl-2-phenyl-7-(phenylmethyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₂₁H₂₀N₄

SR Chemical Library

LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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RN 319481-50-0 REGISTRY

CN 1-Butanol,

2-[[2-(4-chlorophenyl)-5,6-dimethyl-7-[(1*R*)-1-phenylethyl]-7*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl]amino]-
(9*CI*) (CA INDEX NAME)

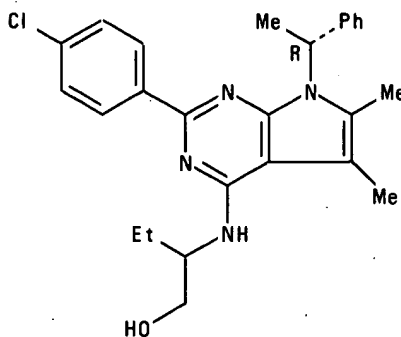
FS STEREOSEARCH

MF C₂₆H₂₉ClN₄O

SR CA

LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry.



***PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

134:100695

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

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L2 ANSWER 114 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 319481-49-7 REGISTRY

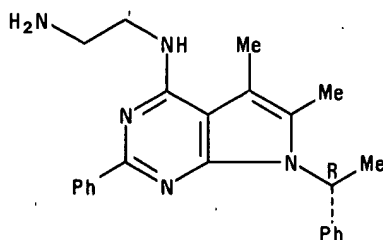
CN 1,2-Ethanediamine, *N*-[5,6-dimethyl-2-phenyl-7-[(1*R*)-1-phenylethyl]-7*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl]-
(9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C₂₄H₂₇N₅

SR CA

LC STN Files: CA, CAPLUS, CASREACT
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

134:100695

L2 ANSWER 115 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 319481-48-6 REGISTRY

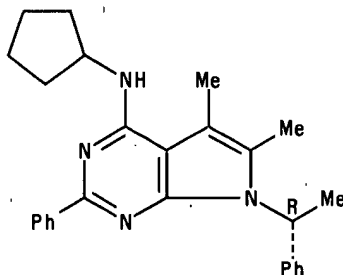
CN 7*H*-Pyrrolo[2,3-*d'*]pyrimidin-4-amine, *N*-cyclopentyl-5,6-dimethyl-2-phenyl-7-[(1*R*)-1-phenylethyl]-
(9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C₂₇H₃₀N₄

SR CA

LC STN Files: CA, CAPLUS, CASREACT
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

134:100695

L2 ANSWER 116 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 319481-47-5 REGISTRY

CN 7*H*-Pyrrolo[2,3-*d'*]pyrimidin-4-amine, 5,6-dimethyl-2-phenyl-*N*,7-bis[(1*R*)-1-phenylethyl]- (9CI) (CA INDEX NAME)

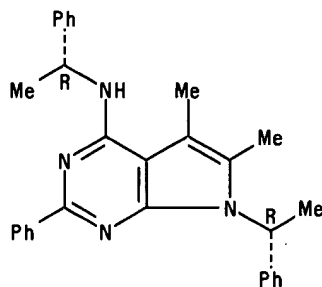
FS STEREOSEARCH

MF C₃₀H₃₀N₄

SR CA

LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

134:100695

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REGISTRY FILE SEARCH RESULTS - P077138C

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L2 ANSWER 117 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 319481-41-9 REGISTRY

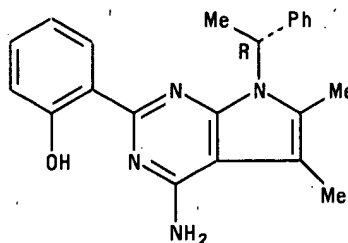
CN Phenol, 2-[4-amino-5,6-dimethyl-7-[(1*R*)-1-phenylethyl]-7*H*-pyrrolo[2,3-*d'*]pyrimidin-2-yl]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C₂₂H₂₂N₄O

SR CA

LC STN Files: CA, CAPLUS, CASREACT
Absolute stereochemistry.



***PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

134:100695

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REGISTRY FILE SEARCH RESULTS - P077138C

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L2 ANSWER 118 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 319481-39-5 REGISTRY

CN 2-Propenoic acid,

3-[[[5,6-dimethyl-7-[(1*R*)-1-phenylethyl]-2-(4-pyridinyl)-7*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl]amino]-, methyl ester (9CI) (CA INDEX NAME)

FS STEREOSEARCH

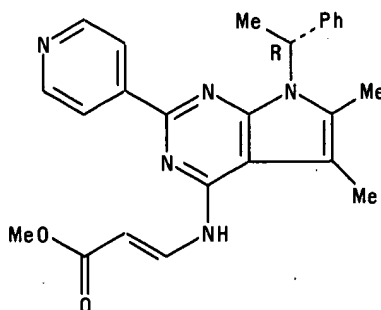
MF C₂₅H₂₅N₅O₂

SR CA

LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry.

Double bond geometry unknown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

134:100695

L2 ANSWER 119 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 319481-26-0 REGISTRY

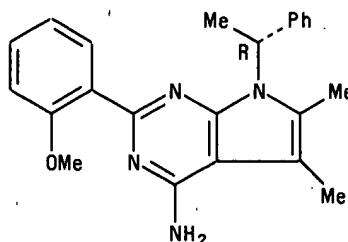
CN 7*H*-Pyrrolo[2,3-*d'*]pyrimidin-4-amine, 2-(2-methoxyphenyl)-5,6-dimethyl-7-[(1*R*)-1-phenylethyl]- (9CI)
(CA INDEX NAME)

FS STEREOSEARCH

MF C₂₃H₂₄N₄O

SR CA

LC STN Files: CA, CAPLUS, CASREACT
Absolute stereochemistry.



***PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

134:100695

L2 ANSWER 120 OF 249 REGISTRY COPYRIGHT 2004 ACS

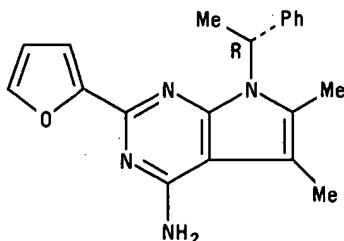
RN 319481-25-9 REGISTRY

CN 7*H*-Pyrrolo[2,3-*d'*]pyrimidin-4-amine, 2-(2-furanyl)-5,6-dimethyl-7-[(1*R*)-1-phenylethyl]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C₂₀H₂₀N₄O

SR CA

LC STN Files: CA, CAPLUS, CASREACT
Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

134:100695

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

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L2 ANSWER 121 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 319481-24-8 REGISTRY

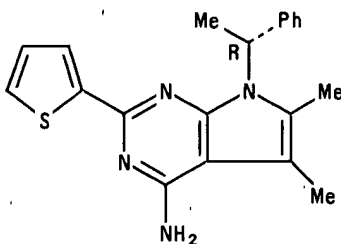
CN 7*H*-Pyrrolo[2,3-*d'*]pyrimidin-4-amine, 5,6-dimethyl-7-[(1*R*)-1-phenylethyl]-2-(2-thienyl)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C₂₀H₂₀N₄S

SR CA

LC STN Files: CA, CAPLUS, CASREACT
Absolute stereochemistry.



****PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT****

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

134:100695

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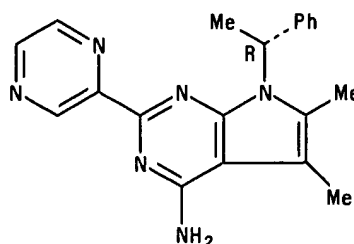
RN 319481-23-7 REGISTRY

CN 7H-Pyrrolo[2,3-d']pyrimidin-4-amine, 5,6-dimethyl-7-[(1*R*)-1-phenylethyl]-2-pyrazinyl- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C₂₀H₂₀N₆

SR CA

LC STN Files: CA, CAPLUS, CASREACT
Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

134:100695

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

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L2 ANSWER 123 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 319481-22-6 REGISTRY

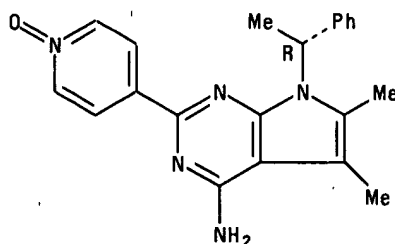
CN 7*H*-Pyrrolo[2,3-*d'*]pyrimidin-4-amine, 5,6-dimethyl-2-(1-oxido-4-pyridinyl)-7-[(1*R*)-1-phenylethyl]- (9CI)
(CA INDEX NAME)

FS STEREOSEARCH

MF C₂₁H₂₁N₅O

SR CA

LC STN Files: CA, CAPLUS, CASREACT
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

134:100695

L2 ANSWER 124 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 319481-21-5 REGISTRY

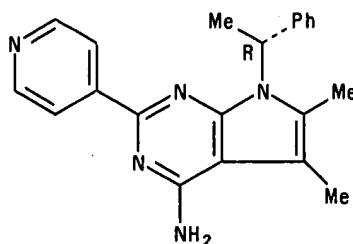
CN 7*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 5,6-dimethyl-7-[(1*R*)-1-phenylethyl]-2-(4-pyridinyl)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C₂₁H₂₁N₅

SR CA

LC STN Files: CA, CAPLUS, CASREACT
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

134:100695

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

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L2 ANSWER 125 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 319481-20-4 REGISTRY

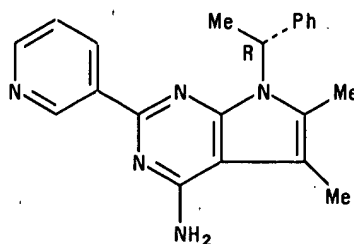
CN 7*H*-Pyrrolo[2,3-*d'*]pyrimidin-4-amine, 5,6-dimethyl-7-[(1*R*)-1-phenylethyl]-2-(3-pyridinyl)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C₂₁H₂₁N₅

SR CA

LC STN Files: CA, CAPLUS, CASREACT
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

134:100695

L2 ANSWER 126 OF 249 REGISTRY COPYRIGHT 2004 ACS

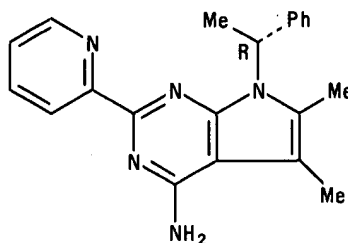
RN 319481-19-1 REGISTRY

CN 7H-Pyrrolo[2,3-d]pyrimidin-4-amine, 5,6-dimethyl-7-[(1*R*)-1-phenylethyl]-2-(2-pyridinyl)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C₂₁H₂₁N₅

SR CA

LC STN Files: CA, CAPLUS, CASREACT
Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

134:100695

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

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L2 ANSWER 127 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251947-24-7 REGISTRY

CN Methanesulfonamide,

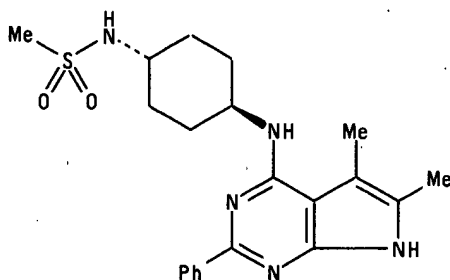
N-[*trans*-4-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]cyclohexyl]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C₂₁H₂₇N₅O₂S

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

10 REFERENCES IN FILE CA (1907 TO DATE)

10 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

139:36534

REFERENCE 4:

138:321287

REFERENCE 5:

138:221598

REFERENCE 6:

137:109485

REFERENCE 7:

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 134

L2 ANSWER 127 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251947-24-7 REGISTRY

137:109288

REFERENCE 8:

136:386128

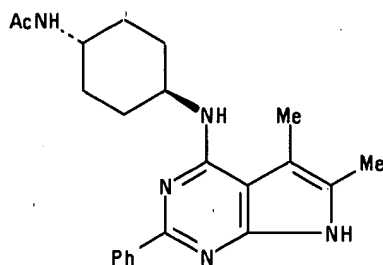
REFERENCE 9:

135:46190

REFERENCE 10:

132:22973

L2 ANSWER 128 OF 249 REGISTRY COPYRIGHT 2004 ACS
RN 251947-22-5 REGISTRY
CN Acetamide, *N*-[*trans*-4-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]cyclohexyl]-
(9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C₂₂H₂₇N₅O
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

10 REFERENCES IN FILE CA (1907 TO DATE)

10 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

139:36534

REFERENCE 4:

138:321287

REFERENCE 5:

138:221598

REFERENCE 6:

137:109485

REFERENCE 7:

137:109288

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REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 136
L2 ANSWER 128 OF 249 REGISTRY COPYRIGHT 2004 ACS
RN 251947-22-5 REGISTRY

REFERENCE 8:

136:386128

REFERENCE 9:

135:46190

REFERENCE 10:

132:22973

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

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L2 ANSWER 129 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-59-5 REGISTRY

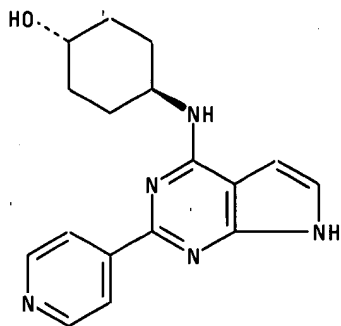
CN Cyclohexanol, 4-[[2-(4-pyridinyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, *trans*- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C₁₇H₁₉N₅O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

STN INTERNATIONAL®

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L2 ANSWER 129 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-59-5 REGISTRY

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

L2 ANSWER 130 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-58-4 REGISTRY

CN Cyclohexanol, 4-[[2-(3-fluorophenyl)-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl]amino]-, *trans*- (9CI) (CA INDEX NAME)

OTHER NAMES:

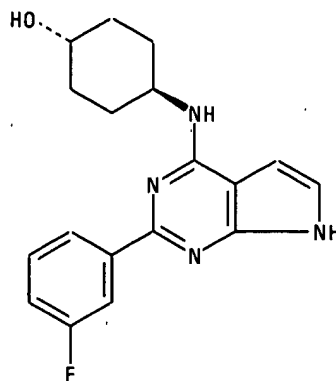
CN 4-[(*trans*-4-Hydroxycyclohexyl)amino]-2-(3-fluorophenyl)-7*H*-pyrrolo[2,3-*d'*]pyrimidine

FS STEREOSEARCH

MF C₁₈H₁₉FN₄O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 140

L2 ANSWER 130 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-58-4 REGISTRY

REFERENCE 6:

137:109288

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

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REGISTRY FILE SEARCH RESULTS - P077138C

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L2 ANSWER 131 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-57-3 REGISTRY

CN Cyclohexanol, 4-[[2-(3-chlorophenyl)-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl]amino]-, *trans*- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 4-[(*trans*-4-Hydroxycyclohexyl)amino]-2-(3-chlorophenyl)-7*H*-pyrrolo[2,3-*d*]pyrimidine

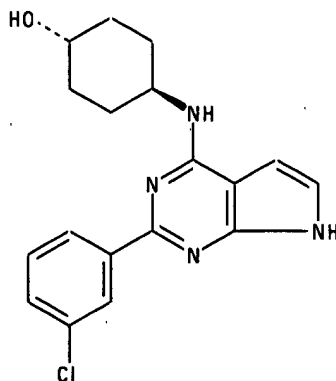
FS STEREOSEARCH

MF C₁₈H₁₉ClN₄O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

STN INTERNATIONAL®

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RN 251946-57-3 REGISTRY

REFERENCE 6:

137:109288

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

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RN 251946-56-2 REGISTRY

CN Urea, *N*-[1-[[[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]methyl]propyl]-*N'*-methyl-
(9CI) (CA INDEX NAME)

OTHER NAMES:

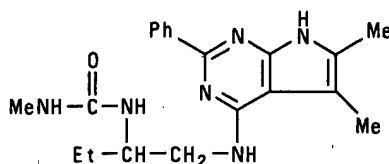
CN 4-[[2-(*N'*-Methylureido)butyl]amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS 3D CONCORD

MF C₂₀H₂₆N₆O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

7 REFERENCES IN FILE CA (1907 TO DATE)

7 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

138:321287

REFERENCE 3:

138:221598

REFERENCE 4:

137:109485

REFERENCE 5:

136:386128

REFERENCE 6:

135:46190

REFERENCE 7:

132:22973

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L2 ANSWER 133 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-55-1 REGISTRY

CN Acetamide, *N*-[1-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]methyl]propyl]- (9CI)
(CA INDEX NAME)

OTHER NAMES:

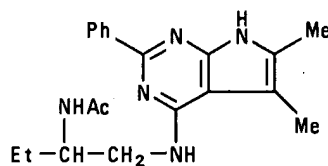
CN 4-[(2-Acetamidobutyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidiné

FS 3D CONCORD

MF C₂₀H₂₅N₅O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

7 REFERENCES IN FILE CA (1907 TO DATE)

7 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

138:321287

REFERENCE 3:

138:221598

REFERENCE 4:

137:109485

REFERENCE 5:

136:386128

REFERENCE 6:

135:46190

REFERENCE 7:

132:22973

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REGISTRY FILE SEARCH RESULTS - P077138C

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RN 251946-54-0 REGISTRY

CN Urea, *N*-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-1-methylethyl]-*N'*-methyl-
(9CI) (CA INDEX NAME)

OTHER NAMES:

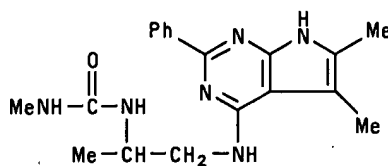
CN 4-[[2-(*N'*-Methylureido)propyl]amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS 3D CONCORD

MF C₁₉H₂₄N₆O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

7 REFERENCES IN FILE CA (1907 TO DATE)

7 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

138:321287

REFERENCE 3:

138:221598

REFERENCE 4:

137:109485

REFERENCE 5:

136:386128

REFERENCE 6:

135:46190

REFERENCE 7:

132:22973

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REGISTRY FILE SEARCH RESULTS - P077138C

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L2 ANSWER 135 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-52-8 REGISTRY

CN Glycine, (1*R*,3*S*)-3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]cyclopentyl ester, *rel*-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C₂₁H₂₅N₅O₂.C₂HF₃O₂

SR CA

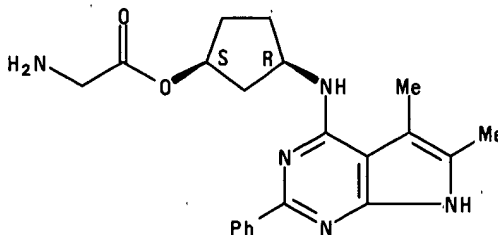
LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

CM 1

CRN 251946-51-7

CMF C₂₁H₂₅N₅O₂

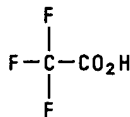
Relative stereochemistry.



CM 2

CRN 76-05-1

CMF C₂HF₃O₂



6 REFERENCES IN FILE CA (1907 TO DATE)

6 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

137:109485

REFERENCE 3:

STN INTERNATIONAL®

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L2 ANSWER 135 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-52-8 REGISTRY

137:109288

REFERENCE 4:

136:386128

REFERENCE 5:

135:46190

REFERENCE 6:

132:22973

L2 ANSWER 136 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-51-7 REGISTRY

CN Glycine, (1*R*,3*S*)-3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]cyclopentyl ester, *rel*- (9CI) (CA INDEX NAME)

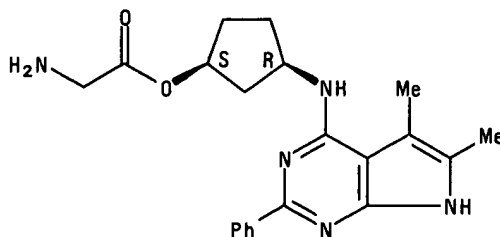
FS STEREOSEARCH

MF C₂₁H₂₅N₅O₂

CI COM

SR CA

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 ANSWER 137 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-50-6 REGISTRY

CN Butanoic acid,

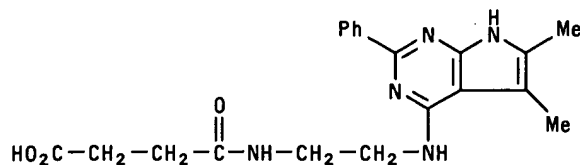
4-[[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]amino]-4-oxo- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₂₀H₂₃N₅O₃

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

8 REFERENCES IN FILE CA (1907 TO DATE)

8 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:221598

REFERENCE 4:

137:109485

REFERENCE 5:

137:109288

REFERENCE 6:

136:386128

REFERENCE 7:

135:46190

REFERENCE 8:

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RN 251946-50-6 REGISTRY
132:22973

L2 ANSWER 138 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-49-3 REGISTRY

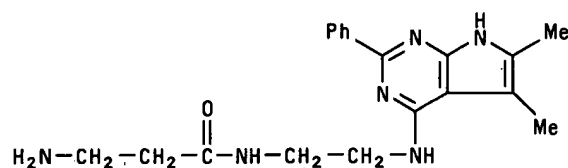
CN Propanamide, 3-amino-*N*-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]ethyl]-
(9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₁₉H₂₄N₆O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

8 REFERENCES IN FILE CA (1907 TO DATE)

8 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:
140:146159

REFERENCE 2:
139:133575

REFERENCE 3:
138:221598

REFERENCE 4:
137:109485

REFERENCE 5:
137:109288

REFERENCE 6:
136:386128

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L2 ANSWER 138 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-49-3 REGISTRY

REFERENCE 7:

135:46190

REFERENCE 8:

132:22973

L2 ANSWER 139 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-48-2 REGISTRY

CN Ethanol, 2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, acetate (ester) (9CI)
(CA INDEX NAME)

OTHER NAMES:

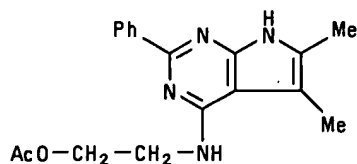
CN 4-[(2-Acetyloxyethyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS 3D CONCORD

MF C₁₈H₂₀N₄O₂

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

STN INTERNATIONAL®

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RN 251946-48-2 REGISTRY

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

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RN 251946-47-1 REGISTRY

CN Acetamide, *N*-[(1*R*,2*R*)-2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]cyclohexyl]-(9CI) (CA INDEX NAME)

OTHER NAMES:

CN (*R,R*)-4-[(2-Acetylamino)cyclohexyl]amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d'*]pyrimidine

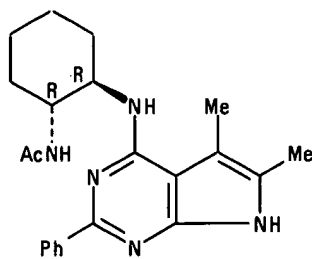
FS STEREOSEARCH

MF C₂₂H₂₇N₅O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 153

L2 ANSWER 140 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-47-1 REGISTRY

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

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L2 ANSWER 141 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-46-0 REGISTRY

CN Acetamide, *N*-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]propyl]- (9CI) (CA INDEX NAME)

OTHER NAMES:

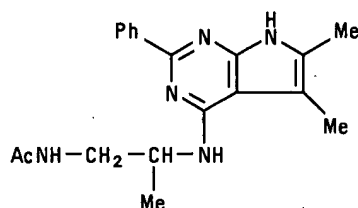
CN 4-[(1-Methyl-2-acetylaminoethyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS 3D CONCORD

MF C₁₉H₂₃N₅O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 155

L2 ANSWER 141 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-46-0 REGISTRY

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

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L2 ANSWER 142 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-45-9 REGISTRY

CN Acetamide, *N*-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-1,1-dimethylethyl]-
(9CI) (CA INDEX NAME)

OTHER NAMES:

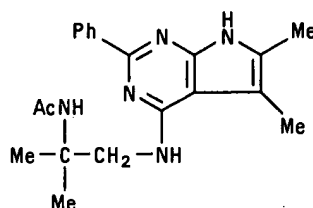
CN 4-[(2-Methyl-2-acetylaminopropyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS 3D CONCORD

MF C₂₀H₂₅N₅O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

STN INTERNATIONAL®

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L2 ANSWER 142 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-45-9 REGISTRY

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

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L2 ANSWER 143 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-44-8 REGISTRY

CN Acetamide, *N*-[(1*S*,2*S*)-2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]cyclohexyl]-(9*CI*) (CA INDEX NAME)

OTHER NAMES:

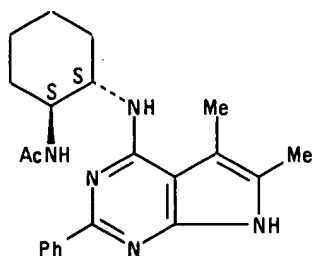
CN (*S,S*)-4-[(2-Acetylaminocyclohexyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS STEREOSEARCH

MF C₂₂H₂₇N₅O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

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REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 159

L2 ANSWER 143 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-44-8 REGISTRY

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

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PAGE 160

L2 ANSWER 144 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-43-7 REGISTRY

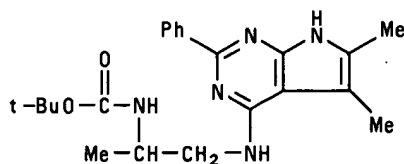
CN Carbamic acid, [2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]-1-methylethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₂₂H₂₉N₅O₂

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

6 REFERENCES IN FILE CA (1907 TO DATE)

6 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

138:321287

REFERENCE 3:

137:109485

REFERENCE 4:

136:386128

REFERENCE 5:

135:46190

REFERENCE 6:

132:22973

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REGISTRY FILE SEARCH RESULTS - P077138C

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RN 251946-42-6 REGISTRY

CN Carbamic acid, [2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]propyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

OTHER NAMES:

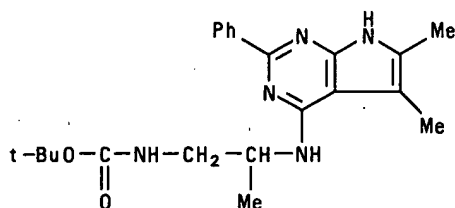
CN 4-[[[1-Methyl-2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d'*]pyrimidine

FS 3D CONCORD

MF C₂₂H₂₉N₅O₂

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 162

L2 ANSWER 145 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-42-6 REGISTRY

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

L2 ANSWER 146 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-41-5 REGISTRY

CN Acetamide, *N*-[(2*S*)-2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]propyl]- (9CI)
(CA INDEX NAME)

OTHER NAMES:

CN (S)-4-[(1-Methyl-2-acetylaminoethyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d'*]pyrimidine

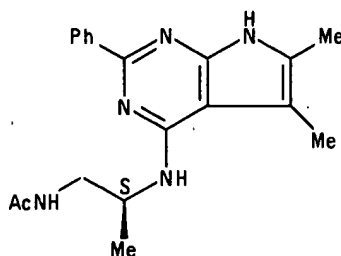
FS STEREOSEARCH

MF C₁₉H₂₃N₅O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 164

L2 ANSWER 146 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-41-5 REGISTRY

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

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RN 251946-40-4 REGISTRY

CN Acetamide, *N*-[(1*S*)-2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-1-methylethyl]-
(9CI) (CA INDEX NAME)

OTHER NAMES:

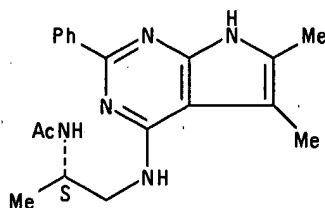
CN (S)-4-[(2-Acetylaminopropyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS STEREOSEARCH

MF C₁₉H₂₃N₅O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 166

L2 ANSWER 147 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-40-4 REGISTRY

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

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L2 ANSWER 148 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-39-1 REGISTRY

CN Acetamide, *N*-[(2*R*)-2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]propyl]- (9CI)
(CA INDEX NAME)

OTHER NAMES:

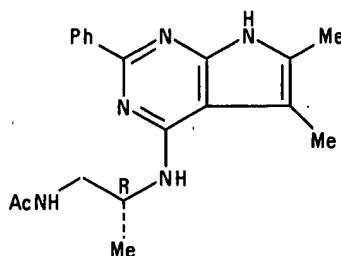
CN (*R*)-4-[(1-Methyl-2-acetylaminoethyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d'*]pyrimidine

FS STEREOSEARCH

MF C₁₉H₂₃N₅O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 168

L2 ANSWER 148 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-39-1 REGISTRY

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

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L2 ANSWER 149 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-38-0 REGISTRY

CN Acetamide, *N*-[(1*R*)-2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-1-methylethyl]-
(9CI) (CA INDEX NAME)

OTHER NAMES:

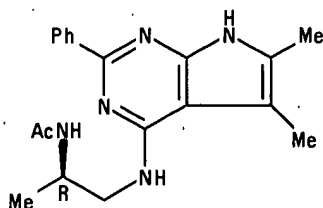
CN (*R*)-4-[(2-Acetylaminopropyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS STEREOSEARCH

MF C₁₉H₂₃N₅O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 170

L2 ANSWER 149 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-38-0 REGISTRY

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

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REGISTRY FILE SEARCH RESULTS - P077138C

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L2 ANSWER 150 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-37-9 REGISTRY

CN Acetamide, *N*-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-1-methylethyl]- (9CI)
(CA INDEX NAME)

OTHER NAMES:

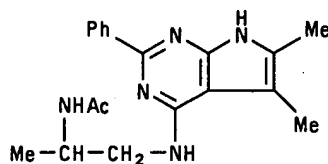
CN 4-[(2-Acetylaminopropyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS 3D CONCORD

MF C₁₉H₂₃N₅O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

136:386128

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L2 ANSWER 150 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-37-9 REGISTRY

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

L2 ANSWER 151 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-36-8 REGISTRY

CN Urea, [2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]- (9CI) (CA INDEX NAME)

OTHER NAMES:

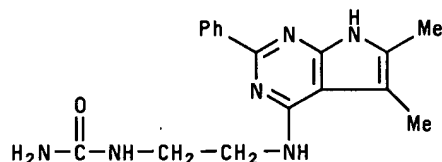
CN 4-[(2-Ureidoethyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS 3D CONCORD

MF C₁₇H₂₀N₆O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 173

L2 ANSWER 151 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-36-8 REGISTRY

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

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L2 ANSWER 152 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-35-7 REGISTRY

CN Propanamide, *N*-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]-2-oxo- (9CI)
(CA INDEX NAME)

OTHER NAMES:

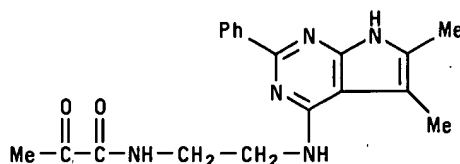
CN 4-[(2-Pyruvylamidoethyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS 3D CONCORD

MF C₁₉H₂₁N₅O₂

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

136:386128

STN INTERNATIONAL®

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L2 ANSWER 152 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-35-7 REGISTRY

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

L2 ANSWER 153 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-34-6 REGISTRY

CN Urea, *N*-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]-*N'*-ethyl- (9CI)
(CA INDEX NAME)

OTHER NAMES:

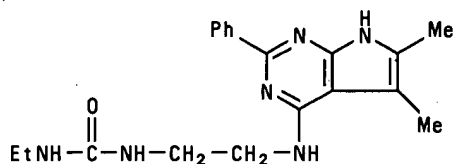
CN 4-[[2-(*N'*-Ethylureido)ethyl]amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS 3D CONCORD

MF C₁₉H₂₄N₆O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

STN INTERNATIONAL®

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L2 ANSWER 153 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-34-6 REGISTRY

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

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L2 ANSWER 154 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-33-5 REGISTRY

CN Urea, *N*-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]-*N'*-methyl- (9CI)
(CA INDEX NAME)

OTHER NAMES:

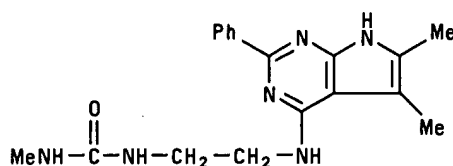
CN 4-[[2-(*N'*-Methylureido)ethyl]amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS 3D CONCORD

MF C₁₈H₂₂N₆O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

136:386128

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RN 251946-33-5 REGISTRY

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

L2 ANSWER 155 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-32-4 REGISTRY

CN Propanamide, *N*-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]- (9CI) (CA INDEX NAME)

OTHER NAMES:

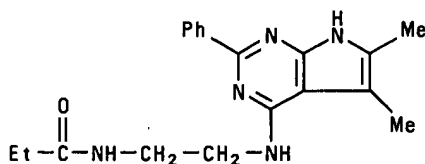
CN 4-[(2-Propionylaminoethyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS 3D CONCORD

MF C₁₉H₂₃N₅O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 179

L2 ANSWER 155 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-32-4 REGISTRY

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

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REGISTRY FILE SEARCH RESULTS - P077138C

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RN 251946-31-3 REGISTRY

CN 1,2-Ethanediamine, *N*-(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)- (9CI) (CA INDEX NAME)

OTHER NAMES:

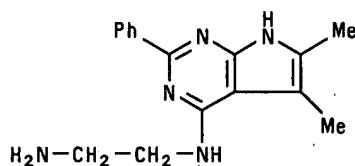
CN 4-[(2-Aminoethyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS 3D CONCORD

MF C₁₆H₁₉N₅

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

136:386128

STN INTERNATIONAL®

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RN 251946-31-3 REGISTRY

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

L2 ANSWER 157 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-30-2 REGISTRY

CN Methanesulfonamide, *N*-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]- (9CI)
(CA INDEX NAME)

OTHER NAMES:

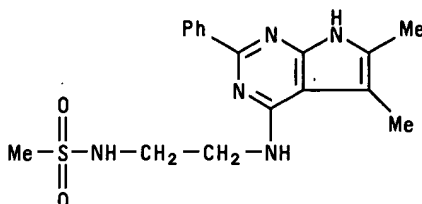
CN 4-[[2-(Methylsulfonylamino)ethyl]amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS 3D CONCORD

MF C₁₇H₂₁N₅O₂S

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



***PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 182
L2 ANSWER 157 OF 249 REGISTRY COPYRIGHT 2004 ACS
RN 251946-30-2 REGISTRY

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

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REGISTRY FILE SEARCH RESULTS - P077138C

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L2 ANSWER 158 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-29-9 REGISTRY

CN Propanamide, *N*-[3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]propyl]- (9CI)
(CA INDEX NAME)

OTHER NAMES:

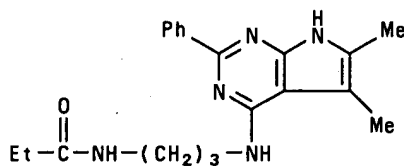
CN 4-[(3-Propionylaminopropyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d'*]pyrimidine

FS 3D CONCORD

MF C₂₀H₂₅N₅O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

136:386128

STN INTERNATIONAL®

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L2 ANSWER 158 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-29-9 REGISTRY

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

L2 ANSWER 159 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-28-8 REGISTRY

CN Propanamide, *N*-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]-2-methyl-
(9CI) (CA INDEX NAME)

OTHER NAMES:

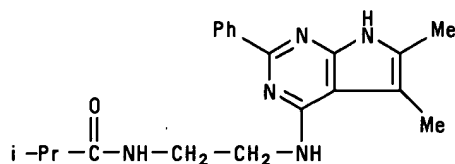
CN 4-[(2-Isobutrylaminoethyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS 3D CONCORD

MF C₂₀H₂₅N₅O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 185

L2 ANSWER 159 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-28-8 REGISTRY

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

L2 ANSWER 160 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-27-7 REGISTRY

CN Cyclopropanecarboxamide, *N*-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]-
(9CI) (CA INDEX NAME)

OTHER NAMES:

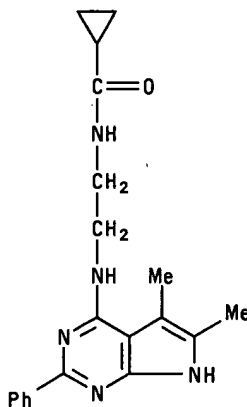
CN 4-[[2-[(Cyclopropanecarbonyl)amino]ethyl]amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS 3D CONCORD

MF C₂₀H₂₃N₅O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

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REFERENCE 5:

137:109485

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REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 187
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RN 251946-27-7 REGISTRY

REFERENCE 6:

137:109288

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

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L2 ANSWER 161 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-26-6 REGISTRY

CN Propanamide, 3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]-*N*-methyl- (9CI)
(CA INDEX NAME)

OTHER NAMES:

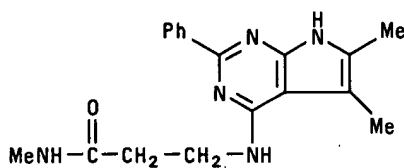
CN 4-[[3-(Methylamino)-3-oxopropyl]amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d'*]pyrimidine

FS 3D CONCORD

MF C₁₈H₂₁N₅O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



****PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT****

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

136:386128

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RN 251946-26-6 REGISTRY

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

L2 ANSWER 162 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-25-5 REGISTRY

CN 1,3-Propanediamine, *N*-(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)- (9CI) (CA INDEX NAME)

OTHER NAMES:

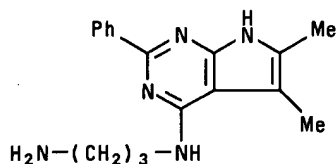
CN 4-[(3-Aminopropyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS 3D CONCORD

MF C₁₇H₂₁N₅

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

8 REFERENCES IN FILE CA (1907 TO DATE)

8 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

138:321287

REFERENCE 3:

138:221598

REFERENCE 4:

137:109485

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REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 190

L2 ANSWER 162 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-25-5 REGISTRY

REFERENCE 5:

137:109288

REFERENCE 6:

136:386128

REFERENCE 7:

135:46190

REFERENCE 8:

132:22973

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

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L2 ANSWER 163 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-24-4 REGISTRY

CN β -Alanine, *N*-(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)- (9CI) (CA INDEX NAME)

OTHER NAMES:

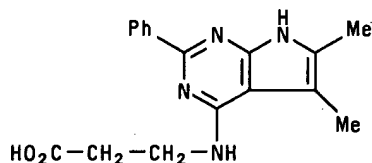
CN 4-[(3-Hydroxy-3-oxopropyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d'*]pyrimidine

FS 3D CONCORD

MF C₁₇H₁₈N₄O₂

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

136:386128

REFERENCE 8:

STN INTERNATIONAL®

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L2 ANSWER 163 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-24-4 REGISTRY

135:46190

REFERENCE 9:

132:22973

L2 ANSWER 164 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-23-3 REGISTRY

CN Acetamide, *N*-[3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]propyl]- (9CI) (CA INDEX NAME)

OTHER NAMES:

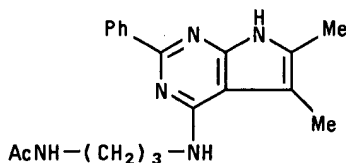
CN 4-[(3-Acetylaminopropyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS 3D CONCORD

MF C₁₉H₂₃N₅O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

STN INTERNATIONAL®

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L2 ANSWER 164 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-23-3 REGISTRY

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

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PAGE 194

L2 ANSWER 165 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-22-2 REGISTRY

CN Formamide, *N*-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]- (9CI) (CA INDEX NAME)

OTHER NAMES:

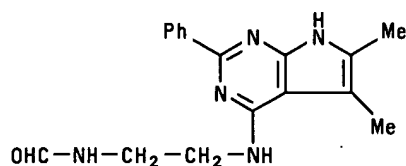
CN 4-[(2-Formylaminoethyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS 3D CONCORD

MF C₁₇H₁₉N₅O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



****PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT****

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

136:386128

STN INTERNATIONAL®

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L2 ANSWER 165 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-22-2 REGISTRY

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

L2 ANSWER 166 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-21-1 REGISTRY

CN Propanamide, 3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-*N,N*-dimethyl- (9CI)
(CA INDEX NAME)

OTHER NAMES:

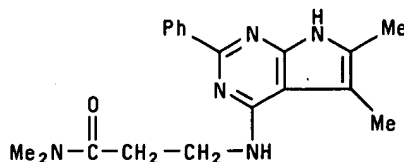
CN 4-[[3-(Dimethylamino)-3-oxopropyl]amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS 3D CONCORD

MF C₁₉H₂₃N₅O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 196

L2 ANSWER 166 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-21-1 REGISTRY

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

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REGISTRY FILE SEARCH RESULTS - P077138C

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L2 ANSWER 167 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-20-0 REGISTRY

CN Cyclohexanol, 4-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]-, *cis*- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 4-[(4-*cis*-Hydroxycyclohexyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d'*]pyrimidine

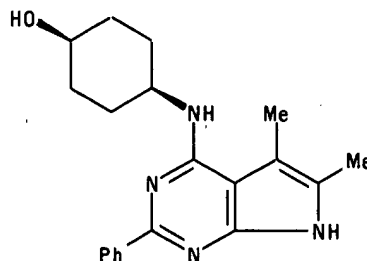
FS STEREOSEARCH

MF C₂₀H₂₄N₄O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

STN INTERNATIONAL®

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L2 ANSWER 167 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-20-0 REGISTRY

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

L2 ANSWER 168 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-19-7 REGISTRY

CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, *N*-3-cyclohexen-1-yl-5,6-dimethyl-2-phenyl- (9CI) (CA INDEX NAME)

OTHER NAMES:

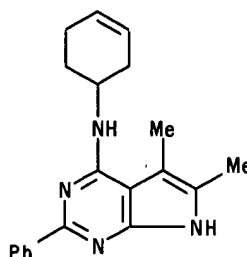
CN 4-[(3-Cyclohexenyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS 3D CONCORD

MF C₂₀H₂₂N₄

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

STN INTERNATIONAL®

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L2 ANSWER 168 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-19-7 REGISTRY

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

L2 ANSWER 169 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-18-6 REGISTRY

CN Cyclohexanol, 4-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, benzoate (ester), *cis*- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 4-[(4-*cis*-Benzoyloxycyclohexyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

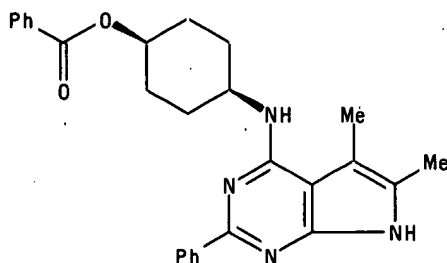
FS STEREOSEARCH

MF C₂₇H₂₈N₄O₂

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

8 REFERENCES IN FILE CA (1907 TO DATE)

8 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

138:321287

REFERENCE 3:

138:221598

REFERENCE 4:

137:109485

REFERENCE 5:

137:109288

REFERENCE 6:

136:386128

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L2 ANSWER 169 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-18-6 REGISTRY

REFERENCE 7:

135:46190

REFERENCE 8:

132:22973

L2 ANSWER 170 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-17-5 REGISTRY

CN 1-Butanol, 4-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]- (9CI) (CA INDEX NAME)

OTHER NAMES:

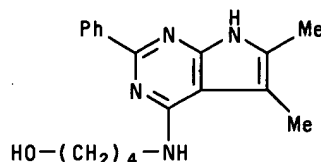
CN 4-[(4-Hydroxybutyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS 3D CONCORD

MF C₁₈H₂₂N₄O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 203

L2 ANSWER 170 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-17-5 REGISTRY

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

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REGISTRY FILE SEARCH RESULTS - P077138C

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L2 ANSWER 171 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-16-4 REGISTRY

CN 1-Propanol, 3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]- (9CI) (CA INDEX NAME)

OTHER NAMES:

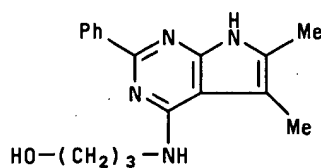
CN 4-[(3-Hydroxypropyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS 3D CONCORD

MF C₁₇H₂₀N₄O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

136:386128

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 205

L2 ANSWER 171 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-16-4 REGISTRY

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

L2 ANSWER 172 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-15-3 REGISTRY

CN Ethanol, 2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]- (9CI) (CA INDEX NAME)

OTHER NAMES:

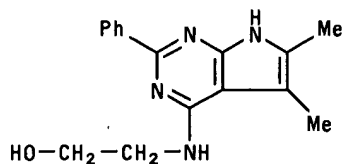
CN 4-[(2-Hydroxyethyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS 3D CONCORD

MF C₁₆H₁₈N₄O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 206

L2 ANSWER 172 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-15-3 REGISTRY

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

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L2 ANSWER 173 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-14-2 REGISTRY

CN β -Alanine, *N*-(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)-, 1,1-dimethylethyl ester (9CI)
(CA INDEX NAME)

OTHER NAMES:

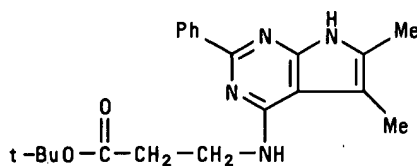
CN 4-[(3-*tert*-Butyloxy-3-oxopropyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d'*]pyrimidine

FS 3D CONCORD

MF C₂₁H₂₆N₄O₂

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

136:386128

STN INTERNATIONAL®

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L2 ANSWER 173 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-14-2 REGISTRY

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

L2 ANSWER 174 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-13-1 REGISTRY

CN Acetamide, 2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-*N*-methyl- (9CI) (CA INDEX NAME)

OTHER NAMES:

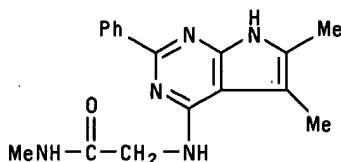
CN 4-[[2-(Methylamino)-2-oxoethyl]amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS 3D CONCORD

MF C₁₇H₁₉N₅O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 209

L2 ANSWER 174 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-13-1 REGISTRY

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

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REGISTRY FILE SEARCH RESULTS - P077138C

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RN 251946-12-0 REGISTRY

CN Acetamide, 2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]- (9CI) (CA INDEX NAME)

OTHER NAMES:

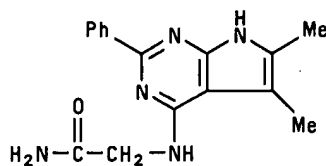
CN 4-[(2-Amino-2-oxoethyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d'*]pyrimidine

FS 3D CONCORD

MF C₁₆H₁₇N₅O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

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138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

136:386128

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 211

L2 ANSWER 175 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-12-0 REGISTRY

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

L2 ANSWER 176 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-11-9 REGISTRY

CN Propanamide, *N*-(cyclopropylmethyl)-3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-
(9CI) (CA INDEX NAME)

OTHER NAMES:

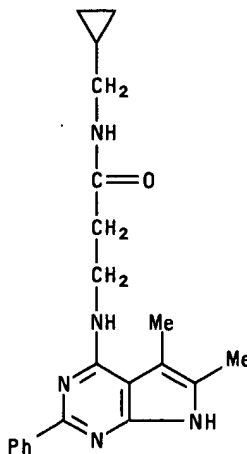
CN 4-[[3-(Cyclopropylmethylamino)-3-oxopropyl]amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS 3D CONCORD

MF C₂₁H₂₅N₅O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

10 REFERENCES IN FILE CA (1907 TO DATE)

10 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 212

L2 ANSWER 176 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-11-9 REGISTRY

139:133575

REFERENCE 3:

139:36534

REFERENCE 4:

138:321287

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REFERENCE 8:

136:386128

REFERENCE 9:

135:46190

REFERENCE 10:

132:22973

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REGISTRY FILE SEARCH RESULTS - P077138C

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RN 251946-10-8 REGISTRY

CN Propanamide, 3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]- (9CI) (CA INDEX NAME)

OTHER NAMES:

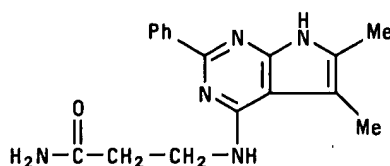
CN 4-[(3-Amino-3-oxopropyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS 3D CONCORD

MF C₁₇H₁₉N₅O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

136:386128

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 214

L2 ANSWER 177 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-10-8 REGISTRY

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

L2 ANSWER 178 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-09-5 REGISTRY

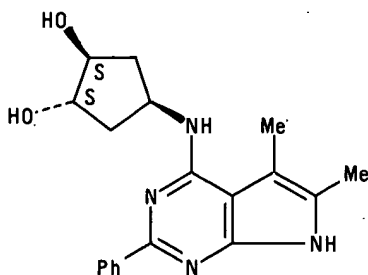
CN 1,2-Cyclopentanediol, 4-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, stereoisomer (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C₁₉H₂₂N₄O₂

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

5 REFERENCES IN FILE CA (1907 TO DATE)

5 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

138:321287

REFERENCE 3:

136:386128

REFERENCE 4:

135:46190

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 215
L2 ANSWER 178 OF 249 REGISTRY COPYRIGHT 2004 ACS
RN 251946-09-5 REGISTRY

REFERENCE 5:

132:22973

L2 ANSWER 179 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-08-4 REGISTRY

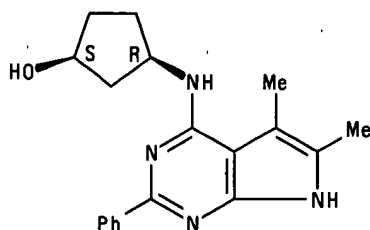
CN Cyclopentanol, 3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, (1*R*,3*S*)-*rel*- (9CI)
(CA INDEX NAME)

FS STEREOSEARCH

MF C₁₉H₂₂N₄O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 216
L2 ANSWER 179 OF 249 REGISTRY COPYRIGHT 2004 ACS
RN 251946-08-4 REGISTRY

REFERENCE 6:

137:109288

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

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L2 ANSWER 180 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-07-3 REGISTRY

CN Cyclopentanol, 3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, (1*R*,3*R*)-*rel*- (9CI)
(CA INDEX NAME)

OTHER NAMES:

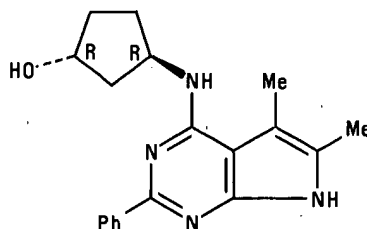
CN 4-[(3-*trans*-Hydroxycyclopentyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS STEREOSEARCH

MF C₁₉H₂₂N₄O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

STN INTERNATIONAL®

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RN 251946-07-3 REGISTRY

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

L2 ANSWER 181 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-06-2 REGISTRY

CN Cyclopentanol, 2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, (1*R*,2*R*)-*rel*- (9CI)
(CA INDEX NAME)

OTHER NAMES:

CN 4-[(2-*trans*-Hydroxycyclopentyl)amino]-5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidine

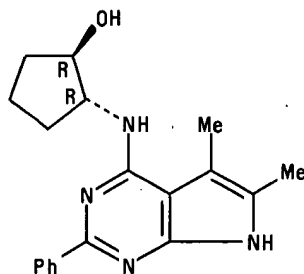
FS STEREOSEARCH

MF C₁₉H₂₂N₄O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 220

L2 ANSWER 181 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-06-2 REGISTRY

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

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L2 ANSWER 182 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-05-1 REGISTRY

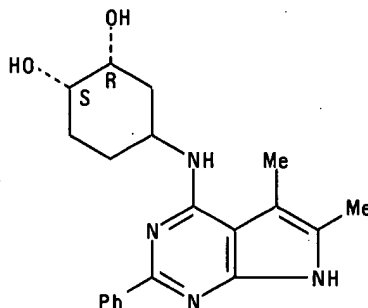
CN 1,2-Cyclohexanediol, 4-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, (1*R*,2*S*)-*rel*-
(9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C₂₀H₂₄N₄O₂

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

5 REFERENCES IN FILE CA (1907 TO DATE)

5 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

138:321287

REFERENCE 3:

136:386128

REFERENCE 4:

135:46190

REFERENCE 5:

132:22973

L2 ANSWER 183 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-04-0 REGISTRY

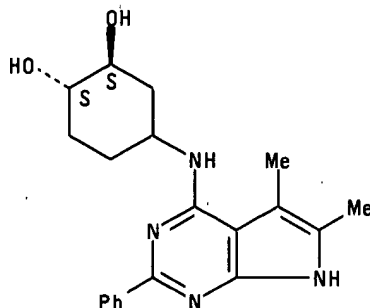
CN 1,2-Cyclohexanediol, 4-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, (1*R*,2*R*)-*rel*-
(9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C₂₀H₂₄N₄O₂

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

5 REFERENCES IN FILE CA (1907 TO DATE)

5 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

138:321287

REFERENCE 3:

136:386128

REFERENCE 4:

135:46190

REFERENCE 5:

132:22973

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

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PAGE 223

L2 ANSWER 184 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-03-9 REGISTRY

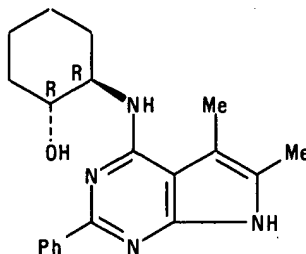
CN Cyclohexanol, 2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]-, (1*R*,2*R*)-*rel*- (9CI)
(CA INDEX NAME)

FS STEREOSEARCH

MF C₂₀H₂₄N₄O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

7 REFERENCES IN FILE CA (1907 TO DATE)

7 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:221598

REFERENCE 4:

137:109288

REFERENCE 5:

136:386128

REFERENCE 6:

135:46190

REFERENCE 7:

132:22973

L2 ANSWER 185 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-01-7 REGISTRY

CN Cyclohexanol, 4-[[2-(2-fluorophenyl)-5,6-dimethyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl]amino]-, *trans*-
(9CI) (CA INDEX NAME)

OTHER NAMES:

CN 4-[(4-*trans*-Hydroxycyclohexyl)amino]-5,6-dimethyl-2-(2-fluorophenyl)-7*H*-pyrrolo[2,3-*d*]pyrimidine

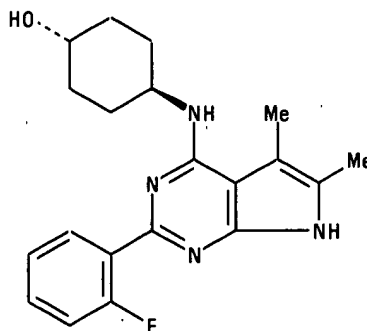
FS STEREOSEARCH

MF C₂₀H₂₃FN₄O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

8 REFERENCES IN FILE CA (1907 TO DATE)

8 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

STN INTERNATIONAL®

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L2 ANSWER 185 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-01-7 REGISTRY

136:386128

REFERENCE 7:

135:46190

REFERENCE 8:

132:22973

L2 ANSWER 186 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-00-6 REGISTRY

CN Cyclohexanol, 4-[[2-(3-fluorophenyl)-5,6-dimethyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl]amino]-, *trans*-
(9CI) (CA INDEX NAME)

OTHER NAMES:

CN 4-[(4-*trans*-Hydroxycyclohexyl)amino]-5,6-dimethyl-2-(3-fluorophenyl)-7*H*-pyrrolo[2,3-*d*]pyrimidine

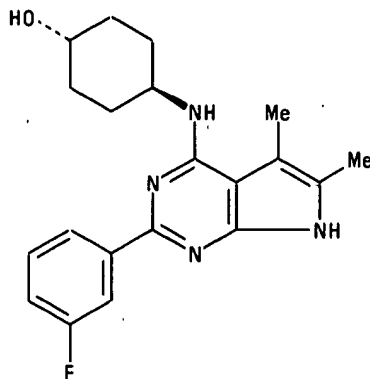
FS STEREOSEARCH

MF C₂₀H₂₃FN₄O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

8 REFERENCES IN FILE CA (1907 TO DATE)

8 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

STN INTERNATIONAL®

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L2 ANSWER 186 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251946-00-6 REGISTRY

REFERENCE 6:

136:386128

REFERENCE 7:

135:46190

REFERENCE 8:

132:22973

L2 ANSWER 187 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251945-99-0 REGISTRY

CN Cyclohexanol, 4-[[2-(4-fluorophenyl)-5,6-dimethyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl]amino]-, *trans*-
(9CI) (CA INDEX NAME)

OTHER NAMES:

CN 4-[(4-*trans*-Hydroxycyclohexyl)amino]-5,6-dimethyl-2-(4-fluorophenyl)-7*H*-pyrrolo[2,3-*d*]pyrimidine

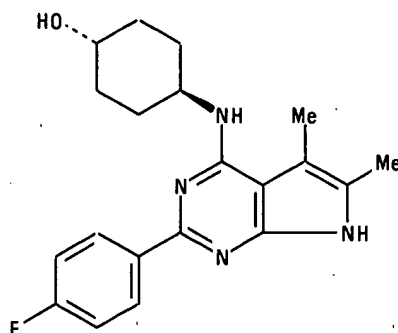
FS STEREOSEARCH

MF C₂₀H₂₃FN₄O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

8 REFERENCES IN FILE CA (1907 TO DATE)

8 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

STN INTERNATIONAL®

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L2 ANSWER 187 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251945-99-0 REGISTRY

136:386128

REFERENCE 7:

135:46190

REFERENCE 8:

132:22973

L2 ANSWER 188 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251945-98-9 REGISTRY

CN Cyclohexanol, 4-[[5,6-dimethyl-2-(3-thienyl)-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl]amino]-, *trans*- (9CI)
(CA INDEX NAME)

OTHER NAMES:

CN 4-[(4-*trans*-Hydroxycyclohexyl)amino]-5,6-dimethyl-2-(3-thienyl)-7*H*-pyrrolo[2,3-*d*]pyrimidine

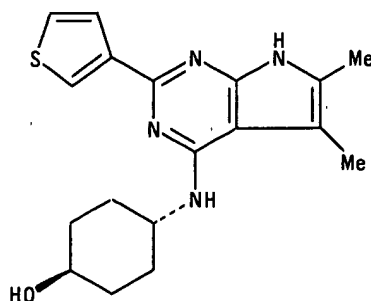
FS STEREOSEARCH

MF C₁₈H₂₂N₄OS

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 231

L2 ANSWER 188 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251945-98-9 REGISTRY

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

L2 ANSWER 189 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251945-97-8 REGISTRY

CN Cyclohexanol, 4-[[5,6-dimethyl-2-(2-thienyl)-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl]amino]-, *trans*- (9CI)
(CA INDEX NAME)

OTHER NAMES:

CN 4-[(4-*trans*-Hydroxycyclohexyl)amino]-5,6-dimethyl-2-(2-thienyl)-7*H*-pyrrolo[2,3-*d'*]pyrimidine

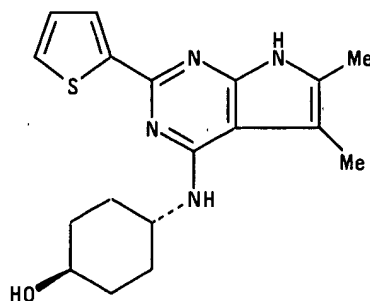
FS STEREOSEARCH

MF C₁₈H₂₂N₄OS

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 233
L2 ANSWER 189 OF 249 REGISTRY COPYRIGHT 2004 ACS
RN 251945-97-8 REGISTRY

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

L2 ANSWER 190 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251945-96-7 REGISTRY

CN Cyclohexanol, 4-[(2-cyclopentyl-5,6-dimethyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, *trans*- (9CI)
(CA INDEX NAME)

OTHER NAMES:

CN 4-[(4-*trans*-Hydroxycyclohexyl)amino]-5,6-dimethyl-2-cyclopentyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

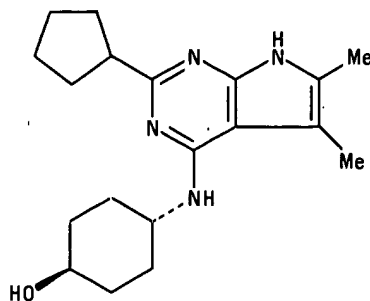
FS STEREOSEARCH

MF C₁₉H₂₈N₄O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

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REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 235
L2 ANSWER 190 OF 249 REGISTRY COPYRIGHT 2004 ACS
RN 251945-96-7 REGISTRY

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

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L2 ANSWER 191 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251945-95-6 REGISTRY

CN Cyclohexanol, 4-[[2-(3-furanyl)-5,6-dimethyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl]amino]-, *trans*- (9CI)
(CA INDEX NAME)

OTHER NAMES:

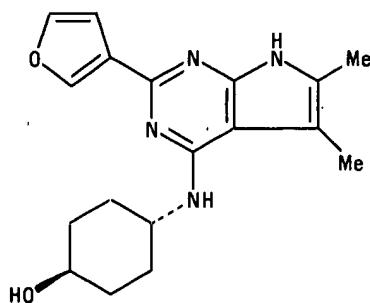
CN 4-[(4-*trans*-Hydroxycyclohexyl)amino]-5,6-dimethyl-2-(3-furyl)-7*H*-pyrrolo[2,3-*d'*]pyrimidine

FS STEREOSEARCH

MF C₁₈H₂₂N₄O₂

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 237
L2 ANSWER 191 OF 249 REGISTRY COPYRIGHT 2004 ACS
RN 251945-95-6 REGISTRY

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 238

L2 ANSWER 192 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251945-94-5 REGISTRY

CN Cyclohexanol, 4-[[2-(2-furanyl)-5,6-dimethyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl]amino]-, *trans*- (9CI)
(CA INDEX NAME)

OTHER NAMES:

CN 4-[(4-*trans*-Hydroxycyclohexyl)amino]-5,6-dimethyl-2-(2-furyl)-7*H*-pyrrolo[2,3-*d*]pyrimidine

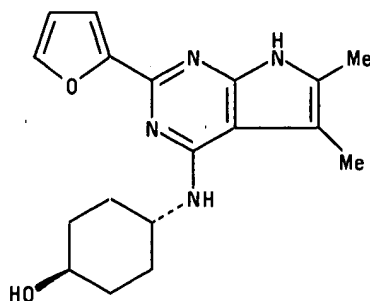
FS STEREOSEARCH

MF C₁₈H₂₂N₄O₂

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 239

L2 ANSWER 192 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251945-94-5 REGISTRY

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

L2 ANSWER 193 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251945-93-4 REGISTRY

CN Cyclohexanol, 4-[[5,6-dimethyl-2-(3-pyridinyl)-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl]amino]-, *trans*- (9CI)
(CA INDEX NAME)

OTHER NAMES:

CN 4-[(4-*trans*-Hydroxycyclohexyl)amino]-5,6-dimethyl-2-(3-pyridyl)-7*H*-pyrrolo[2,3-*d'*]pyrimidine

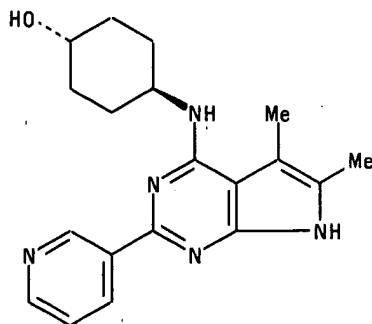
FS STEREOSEARCH

MF C₁₉H₂₃N₅O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

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REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 241
L2 ANSWER 193 OF 249 REGISTRY COPYRIGHT 2004 ACS
RN 251945-93-4 REGISTRY
137:109288

REFERENCE 7:
136:386128

REFERENCE 8:
135:46190

REFERENCE 9:
132:22973

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

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L2 ANSWER 194 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251945-92-3 REGISTRY

CN Cyclohexanol, 4-[(2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, *trans*- (9CI) (CA INDEX NAME)

OTHER NAMES:

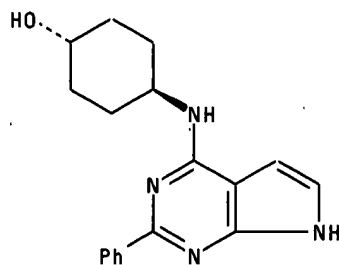
CN 4-[(4-*trans*-Hydroxycyclohexyl)amino]-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS STEREOSEARCH

MF C₁₈H₂₀N₄O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

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REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 243

L2 ANSWER 194 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251945-92-3 REGISTRY

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

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REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

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L2 ANSWER 195 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251945-91-2 REGISTRY

CN Cyclohexanol, 4-[(5-methyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]-, *trans*- (9CI) (CA INDEX NAME)

OTHER NAMES:

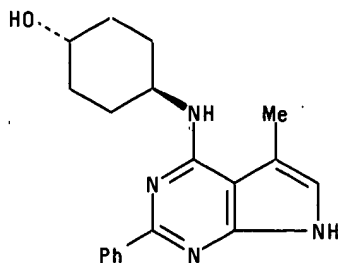
CN 4-[(4-*trans*-Hydroxycyclohexyl)amino]-5-methyl-2-phenyl-7*H*-pyrrolo[2,3-*d'*]pyrimidine

FS STEREOSEARCH

MF C₁₉H₂₂N₄O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 245

L2 ANSWER 195 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251945-91-2 REGISTRY

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 246

L2 ANSWER 196 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251945-90-1 REGISTRY

CN Cyclohexanol, 4-[(6-methyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, *trans*- (9CI) (CA INDEX NAME)

OTHER NAMES:

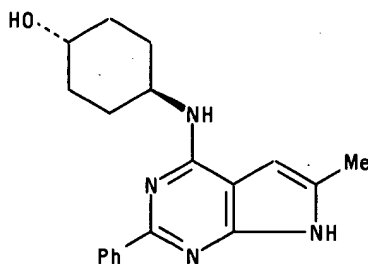
CN 4-[(4-*trans*-Hydroxycyclohexyl)amino]-6-methyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS STEREOSEARCH

MF C₁₉H₂₂N₄O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1907 TO DATE)

9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 247

L2 ANSWER 196 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 251945-90-1 REGISTRY

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

L2 ANSWER 197 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 246855-48-1 REGISTRY

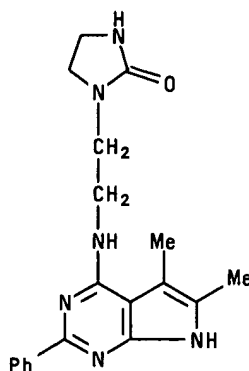
CN 2-Imidazolidinone, 1-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]ethyl]- (9CI)
(CA INDEX NAME)

FS 3D CONCORD

MF C₁₉H₂₂N₆O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

REFERENCE 2:

131:281026

L2 ANSWER 198 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 246855-47-0 REGISTRY

CN 1*H*-Inden-1-ol, 2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-2,3-dihydro-, (1*R*,2*R*)-*rel*- (9CI) (CA INDEX NAME)

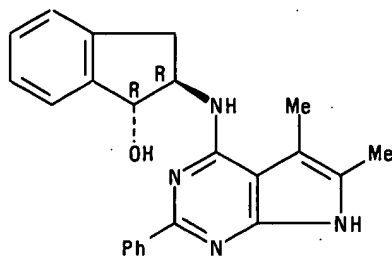
FS STEREOSEARCH

MF C₂₃H₂₂N₄O

SR CA

LC STN Files: CA, CAPLUS

Relative stereochemistry.



****PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT****

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

131:281026

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 249

L2 ANSWER 199 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 246855-46-9 REGISTRY

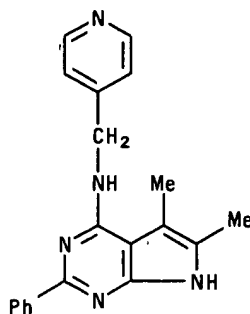
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 5,6-dimethyl-2-phenyl-*N*-(4-pyridinylmethyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₂₀H₁₉N₅

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

REFERENCE 2:

131:281026

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 250

L2 ANSWER 200 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 246855-45-8 REGISTRY

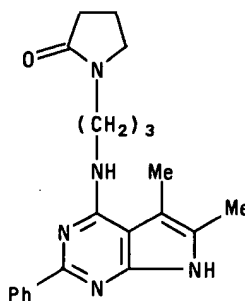
CN 2-Pyrrolidinone, 1-[3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]propyl]- (9CI)
(CA INDEX NAME)

FS 3D CONCORD

MF C₂₁H₂₅N₅O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

REFERENCE 2:

131:281026

L2 ANSWER 201 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 246855-44-7 REGISTRY

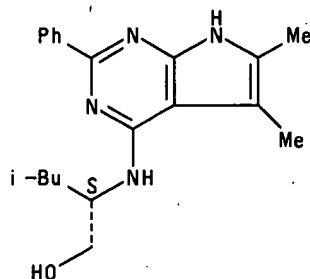
CN 1-Pentanol, 2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]-4-methyl-, (2*S*)- (9CI)
(CA INDEX NAME)

FS STEREOSEARCH

MF C₂₀H₂₆N₄O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

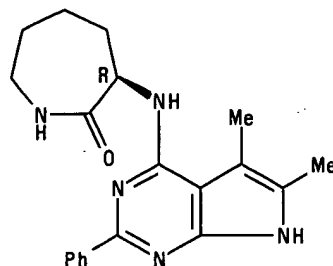
REFERENCE 1:

137:109288

REFERENCE 2:

131:281026

L2 ANSWER 202 OF 249 REGISTRY COPYRIGHT 2004 ACS
 RN 246855-43-6 REGISTRY
 CN 2*H*-Azepin-2-one, 3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d'*]pyrimidin-4-yl)amino]hexahydro-, (3*R*)-
 (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C₂₀H₂₃N₅O
 SR CA
 LC STN Files: CA, CAPLUS
 Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

131:281026

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

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L2 ANSWER 203 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 246855-42-5 REGISTRY

CN Acetamide, *N*-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]- (9CI) (CA INDEX NAME)

OTHER NAMES:

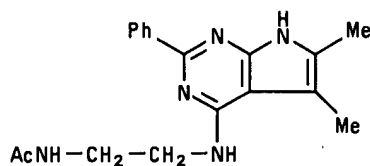
CN 4-[(2-Acetylaminoethyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

FS 3D CONCORD

MF C₁₈H₂₁N₅O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

10 REFERENCES IN FILE CA (1907 TO DATE)

10 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

REFERENCE 7:

136:386128

STN INTERNATIONAL®

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L2 ANSWER 203 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 246855-42-5 REGISTRY

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

REFERENCE 10:

131:281026

L2 ANSWER 204 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 246855-41-4 REGISTRY

CN Cyclohexanol, 4-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, *trans*- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 4-[(4-*trans*-Hydroxycyclohexyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

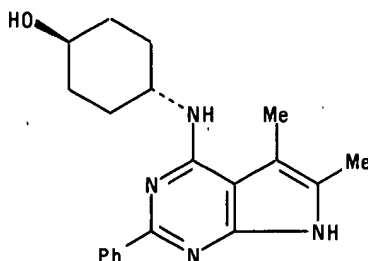
FS STEREOSEARCH

MF C₂₀H₂₄N₄O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

10 REFERENCES IN FILE CA (1907 TO DATE)

10 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

140:146159

REFERENCE 2:

139:133575

REFERENCE 3:

138:321287

REFERENCE 4:

138:221598

REFERENCE 5:

137:109485

REFERENCE 6:

137:109288

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 256

L2 ANSWER 204 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 246855-41-4 REGISTRY

REFERENCE 7:

136:386128

REFERENCE 8:

135:46190

REFERENCE 9:

132:22973

REFERENCE 10:

131:281026

L2 ANSWER 205 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 245488-81-7 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
3-[(4-amino-1H-pyrrolo[2,3-d]pyrimidin-2-yl)thio]-7-[(methoxyacetyl)amino]-8-oxo-, monosodium salt,
(6R,7R)- (9CI) (CA INDEX NAME)

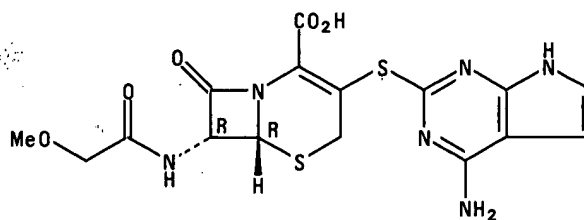
FS STEREOSEARCH

MF C₁₆H₁₆N₆O₅S₂.Na

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.



• Na

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

131:271765

L2 ANSWER 206 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 245488-78-2 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
7-(acetylamino)-3-[(4-amino-1H-pyrrolo[2,3-d]pyrimidin-2-yl)thio]-8-oxo-, monosodium salt, (6R,7R)-
(9CI) (CA INDEX NAME)

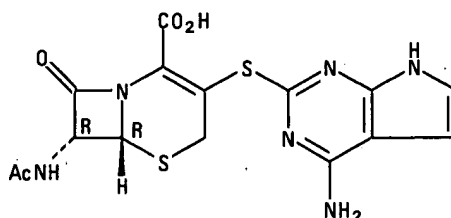
FS STEREOSEARCH

MF C₁₅H₁₄N₆O₄S₂.Na

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.



• Na

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

131:271765

L2 ANSWER 207 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 245488-54-4 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
3-[(4-amino-1*H*-pyrrolo[2,3-*d*]pyrimidin-2-yl)thio]-7-[(methoxyacetyl)amino]-8-oxo-, diphenylmethyl
ester, (6*R*,7*R*)- (9CI) (CA INDEX NAME)

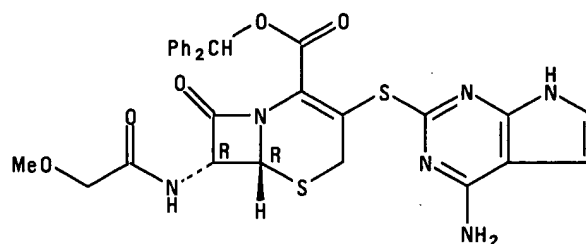
FS STEREOSEARCH

MF C₂₉H₂₆N₆O₅S₂

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

131:271765

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

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L2 ANSWER 208 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 245488-50-0 REGISTRY

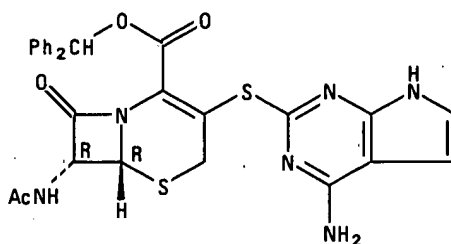
CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
7-(acetylamino)-3-[(4-amino-1*H*-pyrrolo[2,3-*d*]pyrimidin-2-yl)thio]-8-oxo-, diphenylmethyl ester,
(6*R*,7*R*)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C₂₈H₂₄N₆O₄S₂

SR CA

LC STN Files: CA, CAPLUS
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

131:271765

L2 ANSWER 209 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 245488-28-2 REGISTRY

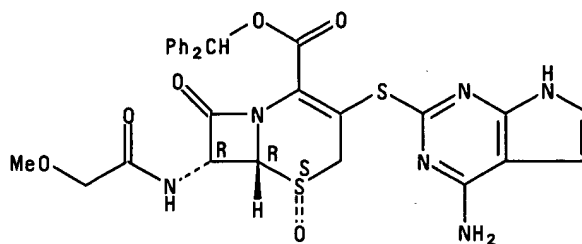
CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
3-[(4-amino-1*H*-pyrrolo[2,3-*d*]pyrimidin-2-yl)thio]-7-[(methoxyacetyl)amino]-8-oxo-, diphenylmethyl
ester, 5-oxide, (5*S*,6*R*,7*R*)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C₂₉H₂₆N₆O₆S₂

SR CA

LC STN Files: CA, CAPLUS
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

131:271765

L2 ANSWER 210 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 245488-25-9 REGISTRY

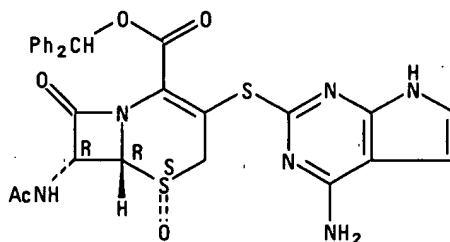
CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
7-(acetylamino)-3-[(4-amino-1*H*-pyrrolo[2,3-*d*]pyrimidin-2-yl)thio]-8-oxo-, diphenylmethyl ester,
5-oxide, (5*S*,6*R*,7*R*)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C₂₈H₂₄N₆O₅S₂

SR CA

LC STN Files: CA, CAPLUS
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

131:271765

L2 ANSWER 211 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 245487-76-7 REGISTRY

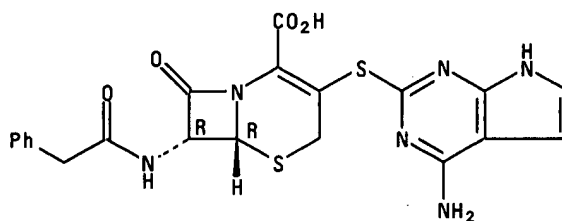
CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
3-[(4-amino-1*H*-pyrrolo[2,3-*d*]pyrimidin-2-yl)thio]-8-oxo-7-[(phenylacetyl)amino]-, monosodium salt,
(6*R*,7*R*)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C₂₁H₁₈N₆O₄S₂.Na

SR CA

LC STN Files: CA, CAPLUS
Absolute stereochemistry.



1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

131:271765

L2 ANSWER 212 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 245487-14-3 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
3-[(4-amino-1*H*-pyrrolo[2,3-*d*]pyrimidin-2-yl)thio]-8-oxo-7-[(phenylacetyl)amino]-, diphenylmethyl
ester, (6*R*,7*R*)- (9CI) (CA INDEX NAME)

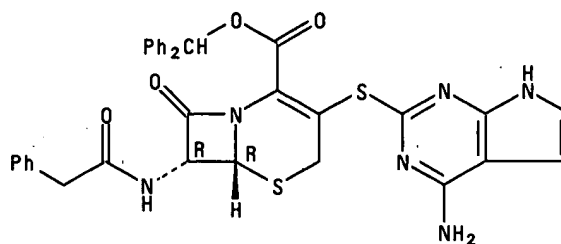
FS STEREOSEARCH

MF C₃₄H₂₈N₆O₄S₂

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

131:271765

L2 ANSWER 213 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 245486-48-0 REGISTRY

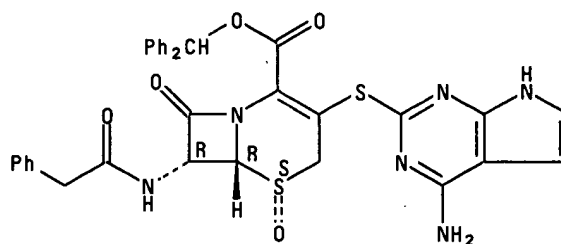
CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
3-[(4-amino-1*H*-pyrrolo[2,3-*d*]pyrimidin-2-yl)thio]-8-oxo-7-[(phenylacetyl)amino]-, diphenylmethyl
ester, 5-oxide, (5*S*,6*R*,7*R*)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C₃₄H₂₈N₆O₅S₂

SR CA

LC STN Files: CA, CAPLUS
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

131:271765

L2 ANSWER 214 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 206197-05-9 REGISTRY

CN 7*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 5,6-dimethyl-7-[(1*R*)-1-methyl-2-phenylethyl]-2-phenyl- (9CI)
(CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 7*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 5,6-dimethyl-7-(1-methyl-2-phenylethyl)-2-phenyl-, (*R*)-

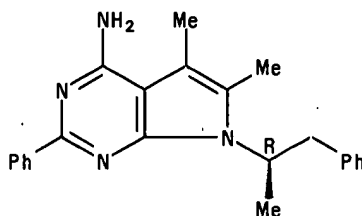
FS STEREOSEARCH

MF C₂₃H₂₄N₄

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

128:299556

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REGISTRY FILE SEARCH RESULTS - P077138C

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L2 ANSWER 215 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 181862-16-8 REGISTRY

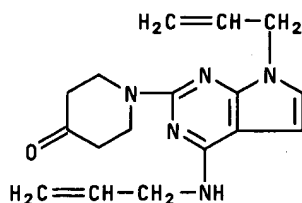
CN 4-Piperidinone, 1-[7-(2-propenyl)-4-(2-propenylamino)-7H-pyrrolo[2,3-d']pyrimidin-2-yl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₁₇H₂₁N₅O

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER



***PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

125:237579

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 267

L2 ANSWER 216 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 181862-15-7 REGISTRY

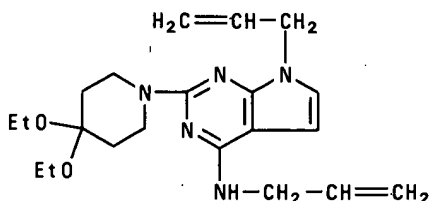
CN 7H-Pyrrolo[2,3-d]pyrimidin-4-amine, 2-(4,4-diethoxy-1-piperidiny)-N,7-di-2-propenyl- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₂₁H₃₁N₅O₂

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

125:237579

L2 ANSWER 217 OF 249 REGISTRY COPYRIGHT 2004 ACS

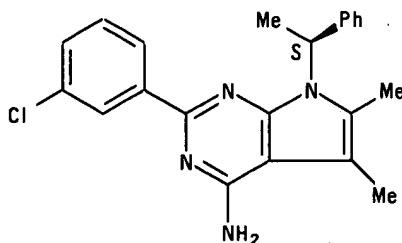
RN 177570-35-3 REGISTRY

CN 7H-Pyrrolo[2,3-d]pyrimidin-4-amine, 2-(3-chlorophenyl)-5,6-dimethyl-7-(1-phenylethyl)-, (S)- (9CI)
(CA INDEX NAME)

FS STEREOSEARCH

MF C₂₂H₂₁ClN₄

SR CA

LC STN Files: CA, CAPLUS
Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

125:25634

L2 ANSWER 218 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 177570-34-2 REGISTRY

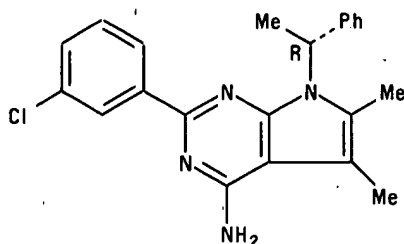
CN 7H-Pyrrolo[2,3-d']pyrimidin-4-amine, 2-(3-chlorophenyl)-5,6-dimethyl-7-(1-phenylethyl)-, (R)- (9CI)
(CA INDEX NAME)

FS STEREOSEARCH

MF C₂₂H₂₁ClN₄

SR CA

LC STN Files: CA, CAPLUS
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

125:25634

L2 ANSWER 219 OF 249 REGISTRY COPYRIGHT 2004 ACS

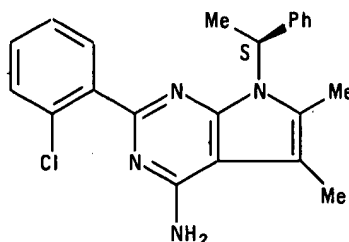
RN 177570-33-1 REGISTRY

CN 7*H*-Pyrrolo[2,3-*d'*]pyrimidin-4-amine, 2-(2-chlorophenyl)-5,6-dimethyl-7-(1-phenylethyl)-, (*S*)- (9CI)
(CA INDEX NAME)

FS STEREOSEARCH

MF C₂₂H₂₁ClN₄

SR CA

LC STN Files: CA, CAPLUS
Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

125:25634

L2 ANSWER 220 OF 249 REGISTRY COPYRIGHT 2004 ACS

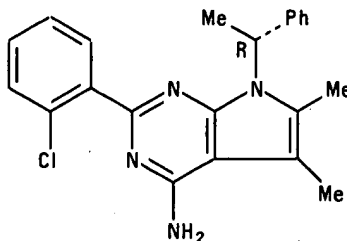
RN 177570-32-0 REGISTRY

CN 7H-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 2-(2-chlorophenyl)-5,6-dimethyl-7-(1-phenylethyl)-, (*R*)- (9CI)
(CA INDEX NAME)

FS STEREOSEARCH

MF C₂₂H₂₁ClN₄

SR CA

LC STN Files: CA, CAPLUS
Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

125:25634

L2 ANSWER 221 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 177499-41-1 REGISTRY

CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 5,6-dimethyl-2-phenyl-*N*-[(1*S*)-1-phenylethyl]- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 5,6-dimethyl-2-phenyl-*N*-(1-phenylethyl)-, (*S*)-

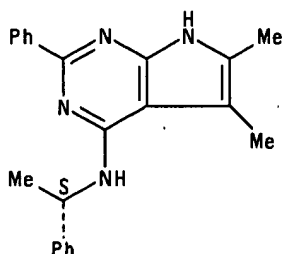
FS STEREOSEARCH

MF C₂₂H₂₂N₄

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

137:109288

REFERENCE 2:

125:25634

L2 ANSWER 222 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 177499-40-0 REGISTRY

CN 1*H*-Pyrrolo[2,3-*d'*]pyrimidin-4-amine, 5,6-dimethyl-2-phenyl-*N*-[(1*R*)-1-phenylethyl]-, (9*CI*) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 1*H*-Pyrrolo[2,3-*d'*]pyrimidin-4-amine, 5,6-dimethyl-2-phenyl-*N*-(1-phenylethyl)-; (*R*)-

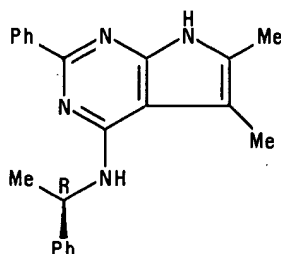
FS STEREOSEARCH

MF C₂₂H₂₂N₄

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

134:100695

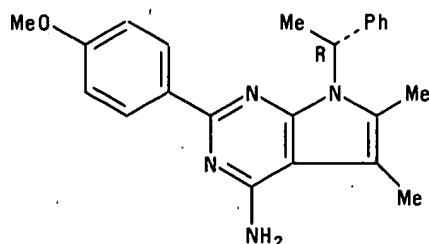
REFERENCE 2:

131:281026

REFERENCE 3:

125:25634

L2 ANSWER 223 OF 249 REGISTRY COPYRIGHT 2004 ACS
RN 177499-37-5 REGISTRY
CN 7*H*-Pyrrolo[2,3-*d'*]pyrimidin-4-amine, 2-(4-methoxyphenyl)-5,6-dimethyl-7-(1-phenylethyl)-, (*R*)- (9CI)
(CA INDEX NAME)
FS STEREOSEARCH
MF C₂₃H₂₄N₄O
SR CA
LC STN Files: CA, CAPLUS
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

125:25634

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

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PAGE 275

L2 ANSWER 224 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 177499-36-4 REGISTRY

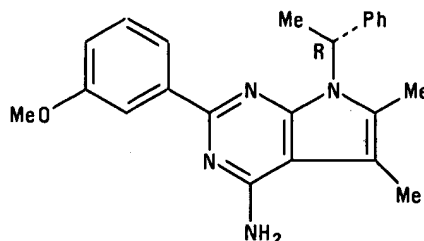
CN 7H-Pyrrolo[2,3-d]pyrimidin-4-amine, 2-(3-methoxyphenyl)-5,6-dimethyl-7-(1-phenylethyl)-, (R)- (9CI)
(CA INDEX NAME)

FS STEREOSEARCH

MF C₂₃H₂₄N₄O

SR CA

LC STN Files: CA, CAPLUS
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

125:25634

L2 ANSWER 225 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 177499-35-3 REGISTRY

CN 7H-Pyrrolo[2,3-d]pyrimidin-4-amine, 2-(3,4-dichlorophenyl)-5,6-dimethyl-7-(1-phenylethyl)-, (S)- (9CI)
(CA INDEX NAME)

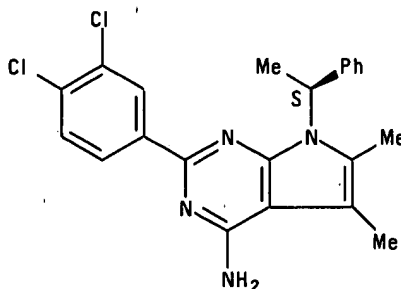
FS STEREOSEARCH

MF C₂₂H₂₀Cl₂N₄

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

125:25634

L2 ANSWER 226 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 177499-34-2 REGISTRY

CN 7*H*-Pyrrolo[2,3-*d'*]pyrimidin-4-amine, 2-(3,4-dichlorophenyl)-5,6-dimethyl-7-(1-phenylethyl)-, (*R*)- (9CI)
(CA INDEX NAME)

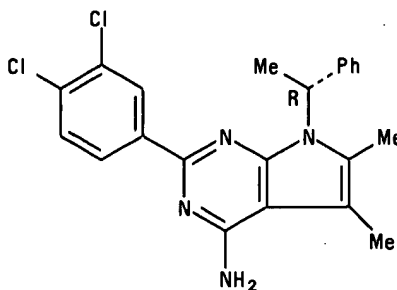
FS STEREOSEARCH

MF C₂₂H₂₀Cl₂N₄

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

125:25634

L2 ANSWER 227 OF 249 REGISTRY COPYRIGHT 2004 ACS

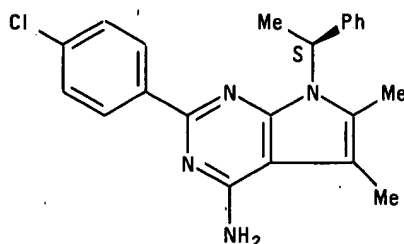
RN 177499-33-1 REGISTRY

CN 7H-Pyrrolo[2,3-d']pyrimidin-4-amine, 2-(4-chlorophenyl)-5,6-dimethyl-7-(1-phenylethyl)-, (S)- (9CI)
(CA INDEX NAME)

FS STEREOSEARCH

MF C₂₂H₂₁ClN₄

SR CA

LC STN Files: CA, CAPLUS
Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

125:25634

L2 ANSWER 228 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 177499-32-0 REGISTRY

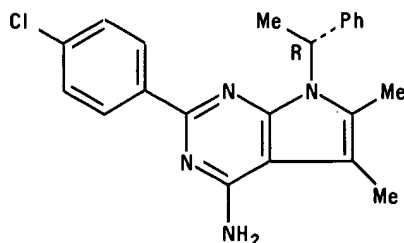
CN 7H-Pyrrolo[2,3-d]pyrimidin-4-amine, 2-(4-chlorophenyl)-5,6-dimethyl-7-(1-phenylethyl)-, (R)- (9CI)
(CA INDEX NAME)

FS STEREOSEARCH

MF C₂₂H₂₁ClN₄

SR CA

LC STN Files: CA, CAPLUS
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

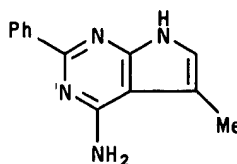
1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

125:25634

L2 ANSWER 229 OF 249 REGISTRY COPYRIGHT 2004 ACS
RN 170170-17-9 REGISTRY
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 5-methyl-2-phenyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C₁₃H₁₂N₄
SR CA
LC STN Files: CA, CAPLUS, CASREACT



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

123:313913

L2 ANSWER 230 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 157838-12-5 REGISTRY

CN 7H-Pyrrolo[2,3-*d*]pyrimidin-4-amine,
2-[4-[[[(10,11-dihydro-5H-dibenzo[*a,d*]cyclohepten-5-yl)methyl]amino]-1-piperidiny]-*N*,7-di-2-propenyl-,
(2*E*)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 7H-Pyrrolo[2,3-*d*]pyrimidin-4-amine,
2-[4-[[[(10,11-dihydro-5H-dibenzo[*a,d*]cyclohepten-5-yl)methyl]amino]-1-piperidiny]-*N*,7-di-2-propenyl-,
(*E*)-2-butenedioate (1:1)

FS STEREOSEARCH

MF C₃₃H₃₈N₆.C₄H₄O₄

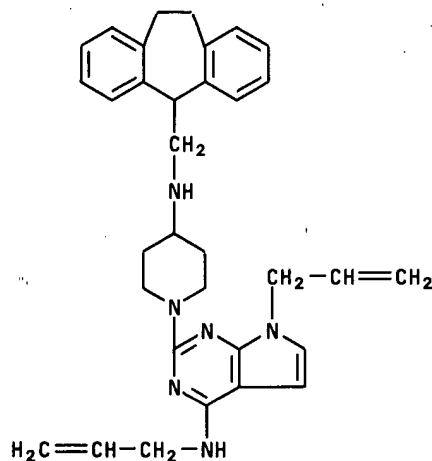
SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

CM 1

CRN 157838-11-4

CMF C₃₃H₃₈N₆

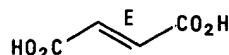


CM 2

CRN 110-17-8

CMF C₄H₄O₄

Double bond geometry as shown.



2 REFERENCES IN FILE CA (1907 TO DATE)

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RN 157838-12-5 REGISTRY

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

125:237579

REFERENCE 2:

121:205381

L2 ANSWER 231 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 157838-11-4 REGISTRY

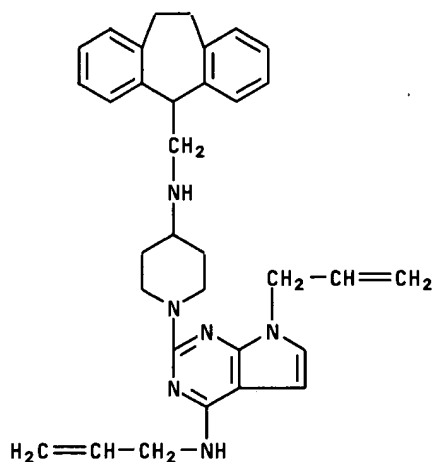
CN 7H-Pyrrolo[2,3-*d*]pyrimidin-4-amine,
2-[4-[[[(10,11-dihydro-5H-dibenzo[*a,d*]cyclohepten-5-yl)methyl]amino]-1-piperidinyl]-N,7-di-2-propenyl-
(9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₃₃H₃₈N₆

CI COM

SR CA



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 ANSWER 232 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 130147-83-0 REGISTRY

CN 7H-Pyrrolo[2,3-d']pyrimidin-4-amine, 2-(3-chlorophenyl)-5,6-dimethyl-7-(1-phenylethyl)- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 7H-Pyrrolo[2,3-d']pyrimidin-4-amine, 2-(3-chlorophenyl)-5,6-dimethyl-7-(1-phenylethyl)-, (±)-

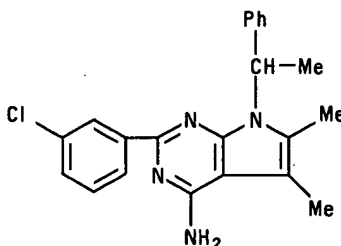
FS 3D CONCORD

MF C₂₂H₂₁ClN₄

SR CA

LC STN Files: BEILSTEIN*, CA, CAPLUS

(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

113:211696

L2 ANSWER 233 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 130147-82-9 REGISTRY

CN 7H-Pyrrolo[2,3-d]pyrimidin-4-amine, 2-(2-chlorophenyl)-5,6-dimethyl-7-(1-phenylethyl)- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 7H-Pyrrolo[2,3-d]pyrimidin-4-amine, 2-(2-chlorophenyl)-5,6-dimethyl-7-(1-phenylethyl)-, (±)-

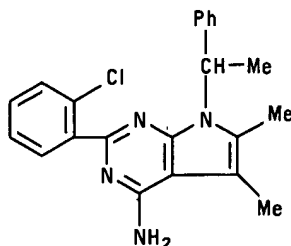
FS 3D CONCORD

MF C₂₂H₂₁ClN₄

SR CA

LC STN Files: BEILSTEIN*, CA, CAPLUS

(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

113:211696

L2 ANSWER 234 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 130147-81-8 REGISTRY

CN 7*H*-Pyrrolo[2,3-*d'*]pyrimidin-4-amine, 5,6-dimethyl-2-phenyl-7-(1-phenylethyl)-, (*S*)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

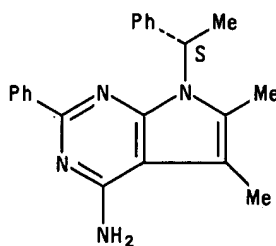
MF C₂₂H₂₂N₄

SR CA

LC STN Files: BEILSTEIN*, CA, CAPLUS

(*File contains numerically searchable property data)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

125:25634

REFERENCE 2:

113:211696

L2 ANSWER 235 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 130147-80-7 REGISTRY

CN 7*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 5,6-dimethyl-2-phenyl-7-[(1*R*)-1-phenylethyl]- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 7*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 5,6-dimethyl-2-phenyl-7-(1-phenylethyl)-, (*R*)-

FS STEREOSEARCH

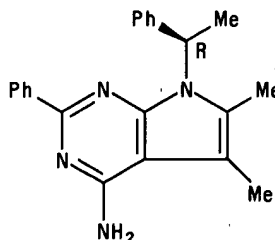
MF C₂₂H₂₂N₄

SR CA

LC STN Files: BEILSTEIN*, CA, CAPLUS, USPAT2, USPATFULL

(*File contains numerically searchable property data)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

7 REFERENCES IN FILE CA (1907 TO DATE)

7 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

134:100695

REFERENCE 2:

130:71627

REFERENCE 3:

127:156859

REFERENCE 4:

125:157747

REFERENCE 5:

125:157746

REFERENCE 6:

125:25634

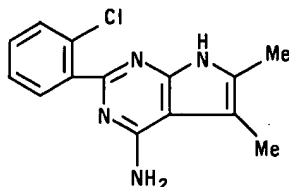
STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C 17 MAR 2004 20:03:18 PAGE 287
L2 ANSWER 235 OF 249 REGISTRY COPYRIGHT 2004 ACS
RN 130147-80-7 REGISTRY

REFERENCE 7:

113:211696

L2 ANSWER 236 OF 249 REGISTRY COPYRIGHT 2004 ACS
RN 130147-79-4 REGISTRY
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 2-(2-chlorophenyl)-5,6-dimethyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C₁₄H₁₃ClN₄
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

127:156859

REFERENCE 2:

113:211696

STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

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L2 ANSWER 237 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 130147-78-3 REGISTRY

CN 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 2-(3-chlorophenyl)-5,6-dimethyl- (9CI) (CA INDEX NAME)

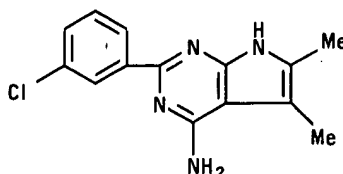
FS 3D CONCORD

MF C₁₄H₁₃ClN₄

SR CA

LC STN Files: BEILSTEIN*, CA, CAPLUS

(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

113:211696

L2 ANSWER 238 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 116673-09-7 REGISTRY

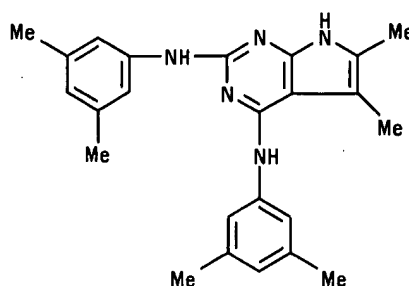
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidine-2,4-diamine, *N,N'*-bis(3,5-dimethylphenyl)-5,6-dimethyl- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₂₄H₂₇N₅

SR CA

LC STN Files: CA, CAPLUS, CASREACT, SPECINFO



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

109:149471

L2 ANSWER 239 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 116673-08-6 REGISTRY

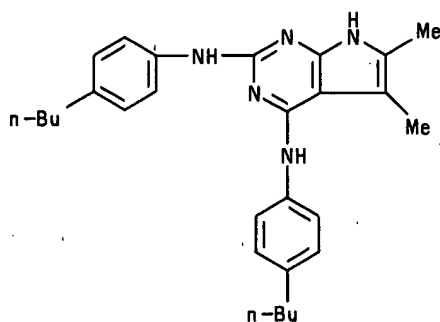
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidine-2,4-diamine, *N,N'*-bis(4-butylphenyl)-5,6-dimethyl- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₂₈H₃₅N₅

SR CA

LC STN Files: CA, CAPLUS, CASREACT, SPECINFO



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

109:149471

L2 ANSWER 240 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 116673-07-5 REGISTRY

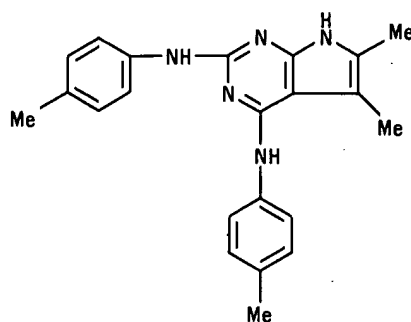
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidine-2,4-diamine, 5,6-dimethyl-*N,N'*-bis(4-methylphenyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₂₂H₂₃N₅

SR CA

LC STN Files: CA, CAPLUS, CASREACT, SPECINFO



****PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT****

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

109:149471

L2 ANSWER 241 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 116673-06-4 REGISTRY

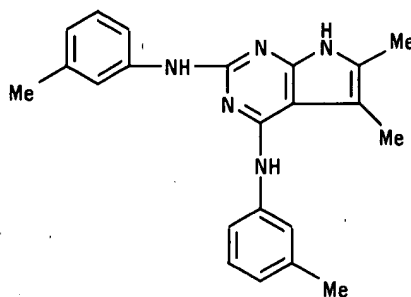
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidine-2,4-diamine, 5,6-dimethyl-*N,N'*-bis(3-methylphenyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₂₂H₂₃N₅

SR CA

LC STN Files: CA, CAPLUS, CASREACT, SPECINFO



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

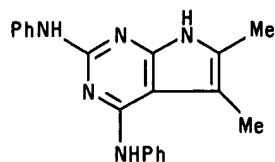
1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

109:149471

L2 ANSWER 242 OF 249 REGISTRY COPYRIGHT 2004 ACS
RN 116673-05-3 REGISTRY
CN 1*H*-Pyrrolo[2,3-*d*]pyrimidine-2,4-diamine, 5,6-dimethyl-*N,N'*-diphenyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C₂₀H₁₉N₅
SR CA
LC STN Files: CA, CAPLUS, CASREACT, SPECINFO



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

109:149471

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REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 294

L2 ANSWER 243 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 111601-40-2 REGISTRY

CN 1*H*-Pyrrolo[2,3-*d'*]pyrimidin-4-amine, 2-(4-chlorophenyl)-5,6-dimethyl- (9CI) (CA INDEX NAME)

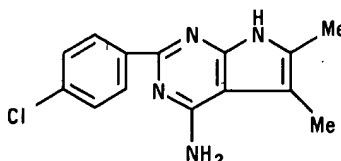
FS 3D CONCORD

MF C₁₄H₁₃ClN₄

SR CA

LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT

(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

113:211696

REFERENCE 2:

107:236656

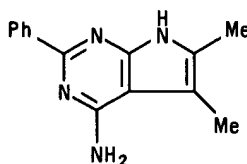
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REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

PAGE 295

L2 ANSWER 244 OF 249 REGISTRY COPYRIGHT 2004 ACS
RN 111601-39-9 REGISTRY
CN 1H-Pyrrolo[2,3-d]pyrimidin-4-amine, 5,6-dimethyl-2-phenyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C₁₄H₁₄N₄
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, TOXCENTER
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

124:249637

REFERENCE 2:

113:211696

REFERENCE 3:

107:236656

L2 ANSWER 245 OF 249 REGISTRY COPYRIGHT 2004 ACS

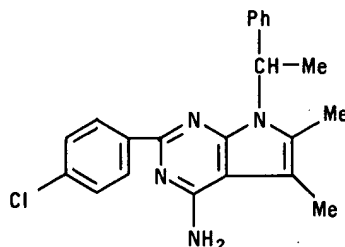
RN 111601-37-7 REGISTRY

CN 7H-Pyrrolo[2,3-d]pyrimidin-4-amine, 2-(4-chlorophenyl)-5,6-dimethyl-7-(1-phenylethyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₂₂H₂₁N₄

SR CA

LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT
(*File contains numerically searchable property data)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

107:236656

L2 ANSWER 246 OF 249 REGISTRY COPYRIGHT 2004 ACS

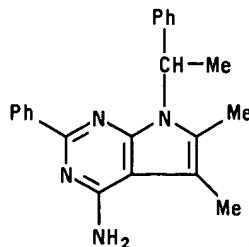
RN 111601-36-6 REGISTRY

CN 7H-Pyrrolo[2,3-d]pyrimidin-4-amine, 5,6-dimethyl-2-phenyl-7-(1-phenylethyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₂₂H₂₂N₄

SR CA

LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT
(*File contains numerically searchable property data)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

107:236656

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REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

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L2 ANSWER 247 OF 249 REGISTRY COPYRIGHT 2004 ACS

RN 94966-89-9 REGISTRY

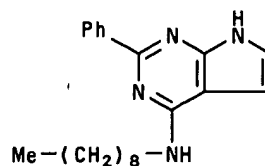
CN 7H-Pyrrolo[2,3-d']pyrimidine, 4-(nonylamino)-2-phenyl- (7CI) (CA INDEX NAME)

FS 3D CONCORD

MF C₂₁H₂₈N₄

LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, TOXCENTER

(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1:

57:76026

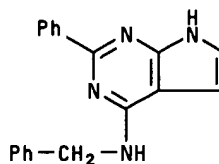
STN INTERNATIONAL®

REGISTRY FILE SEARCH RESULTS - P077138C

17 MAR 2004 20:03:18

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L2 ANSWER 248 OF 249 REGISTRY COPYRIGHT 2004 ACS
RN 94304-61-7 REGISTRY
CN 7H-Pyrrolo[2,3-d]pyrimidine, 4-(benzylamino)-2-phenyl- (7CI) (CA INDEX NAME)
FS 3D CONCORD
MF C₁₉H₁₆N₄
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS
(*File contains numerically searchable property data).



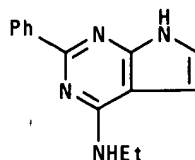
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1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1:

56:46024

L2 ANSWER 249 OF 249 REGISTRY COPYRIGHT 2004 ACS
 RN 92193-06-1 REGISTRY
 CN 7*H*-Pyrrolo[2,3-*d'*]pyrimidine, 4-(ethylamino)-2-phenyl- (7CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C₁₄H₁₄N₄
 LC STN Files: CA, CAOLD, CAPLUS



****PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT****

1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
 1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1:

56:46024

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REQUEST NUMBER: P077139C

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ALEXANDRIA, VA 22314

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Display

Code	Definition
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OREF	Original Reference Number
ED	Entry Date
TI	Title of Document
AU	Author
IN	Patent Inventor
CS	Corporate Source
PA	Patent Assignee
SO	Source
JT	Journal Title
PB	Publisher
PUI	Publisher Item Identifier
URL	Uniform Resource Locator
DT	Document Type
LA	Language
IC	International Patent Classification (IPC)
ICM	Main IPC
ICS	Secondary IPC
ICA	Additional or Supplementary IPC
ICI	Index or Complementary IPC
NCL	National Patent Classification Code
CC	Classification Code (CA Section Code and Title and

CA Section Cross-Reference Code)

FAN.CNT	Family Accession Number Count
CY.CNT	Patent Country Count
PN.CNT	Patent Number Count
PI	Patent Information or Patent Family Table
DS	Designated States (patent)
AI	Patent Application Information
PRAI	Priority Application Information
PY	Publication Year
FAN	Family Accession Number
OS	Other Source
GI	Graphic Image
AB	Abstract
ST	Supplementary Term (CA Keywords)
IT	Index Term
RL	Role
REC.CNT	Cited References Count
RE	Cited References
RETABLE	Cited References Table

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HCAPLUS FILE SEARCH STATISTICS - P077139C

17 MAR 2004 20:04:18 PAGE

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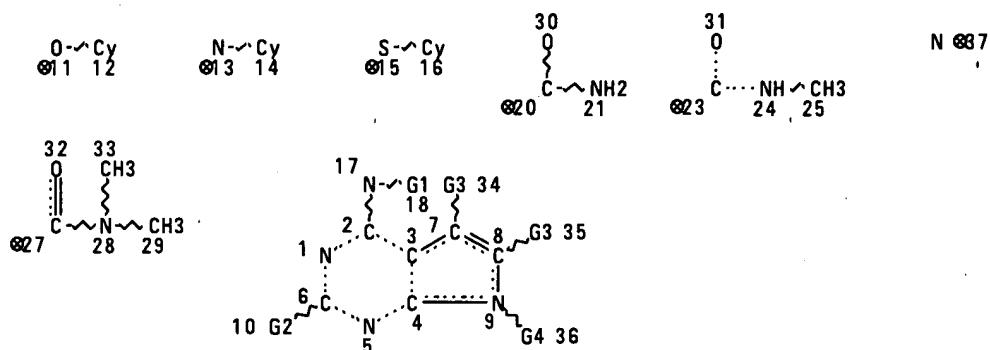
30 ANSWERS PRINTED IN FORMAT 'ED IBIB ABS HITRN'

IN FILE 'HCAPLUS'

USING QUERY:

L1

STR



VAR G1=H/CH3/20/23/27

VAR G2=11/13/15/CY

VAR G3=H/CH3

VAR G4=C/37/H

NODE ATTRIBUTES:

NSPEC IS R AT 37

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC I

NUMBER OF NODES IS 34

STEREO ATTRIBUTES: NONE

L2 249 SEA FILE=REGISTRY SSS FUL L1

L3 30 SEA FILE=HCAPLUS L2

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HCAPLUS FILE SEARCH RESULTS - P077139C

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PAGE

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L3 ANSWER 1 OF 30 HCAPLUS COPYRIGHT 2004 ACS

ED Entered STN: 04 Feb 2004

ACCESSION NUMBER: 2004:88297 HCAPLUS

DOCUMENT NUMBER: 140:146159

TITLE: Preparation and use of substituted pyrrolo[2,3-d]pyrimidines as selective adenosine A₃ receptor antagonists

INVENTOR(S): Castelhana, Arlindo L.; McKibben, Bryan; Witter, David J.

PATENT ASSIGNEE(S): OSI Pharmaceuticals, Inc., USA

SOURCE: U.S., 71 pp., Cont.-in-part of Appl. No. PCT/US99/12135.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6686366	B1	20040203	US 1999-454075	19991202
WO 9962518	A1	19991209	WO 1999-US12135	19990601

W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

WO 2001039777	A1	20010607	WO 2000-US32702	20001201
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W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

EP 1246623	A1	20021009	EP 2000-988011	20001201
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R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR

L3 ANSWER 1 OF 30 HCAPLUS COPYRIGHT 2004 ACS

JP 2003519102

T2

20030617

JP 2001-541509

20001201

PRIORITY APPLN. INFO.:

US 1998-87702P P 19980602

US 1999-123216P P 19990308

US 1999-126527P P 19990326

WO 1999-US12135 A2 19990601

US 1999-454074 A 19991202

US 1999-454075 A 19991202

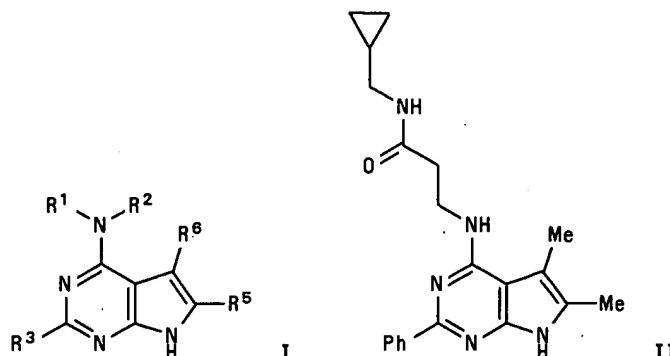
US 1999-454254 A 19991202

WO 2000-US32702 W 20001201

OTHER SOURCE(S):

MARPAT 140:146159

GI



AB The title compds. [I; R¹ = H and R² = cyclopropylmethylaminocarbonylethyl, cis-3-hydroxycyclopentyl, acetamidobutyl, etc.; or NR¹R² = 3-acetamidopiperadino, 3-hydroxypyrrolidino, 3-methoxycarbonylmethylpyrrolidino, etc.; R³ = (un)substituted cycloalkyl, aryl; R⁵ = H, alkyl, aryl; R⁶ = H, alkyl, cycloalkyl] which specifically inhibit the adenosine A₃ receptor and are useful for treating a disease assocd. with A₃ adenosine receptor, were prepd. Thus, 4-chloro-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-d]pyrimidine was reacted with 4-trans-hydroxycyclohexylamine in DMSO at 130°C for 5 h to yield I [R¹ = H; R² = trans-4-hydroxycyclohexyl; R³ = Ph; R⁵, R⁶ = Me] in 75% yield after purifn. which showed K_i of 13.9 nM against adenosine receptor A₁ binding. Some of the compds. I such as II exhibited at least 10 times more selective binding to adenosine receptor A₃ than other receptor subtype. Claimed uses of I includes administration of a systemic formulation (i.e. ophthalmic) for the treatment of a disease assocd. with A₃ adenosine receptors in a subject.

IT ***251946-19-7P***

RL: BYP (Byproduct); PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant)

L3 ANSWER 1 OF 30 HCAPLUS COPYRIGHT 2004 ACS

or reagent); USES (Uses)

(prepn. and use of substituted 7H-pyrrolo[2,3-d]pyrimidines as selective adenosine A₃ receptor antagonists)

IT ***251946-18-6P***

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(prepn. and use of substituted 7H-pyrrolo[2,3-d]pyrimidines as selective adenosine A₃ receptor antagonists)

IT	***246855-41-4P***	***246855-42-5P***	***251945-90-1P***
	251945-91-2P	***251945-92-3P***	***251945-93-4P***
	251945-94-5P	***251945-95-6P***	***251945-96-7P***
	251945-97-8P	***251945-98-9P***	***251945-99-0P***
	251946-00-6P	***251946-01-7P***	***251946-03-9P***
	251946-04-0P	***251946-05-1P***	***251946-06-2P***
	251946-07-3P	***251946-08-4P***	***251946-09-5P***
	251946-10-8P	***251946-11-9P***	***251946-12-0P***
	251946-13-1P	***251946-14-2P***	***251946-15-3P***
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	251946-21-1P	***251946-22-2P***	***251946-23-3P***
	251946-24-4P	***251946-25-5P***	***251946-26-6P***
	251946-27-7P	***251946-28-8P***	***251946-29-9P***
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	343631-99-2P	***343632-03-1P***	***343632-04-2P***
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L3 ANSWER 1 OF 30 HCAPLUS COPYRIGHT 2004 ACS

343632-50-8P ***343632-70-2P*** ***343632-71-3P***

343632-72-4P ***343632-73-5P*** ***343632-77-9P***

343632-78-0P ***343632-79-1P*** ***343633-16-9P***

343969-79-9P ***343969-97-1P***

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. and use of substituted 7H-pyrrolo[2,3-d]pyrimidines as selective adenosine A₃ receptor antagonists)

IT ***343632-96-2P*** ***343632-97-3P***

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and use of substituted 7H-pyrrolo[2,3-d]pyrimidines as selective adenosine A₃ receptor antagonists)

REFERENCE COUNT: 128 THERE ARE 128 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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17 MAR 2004 20:04:19

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8

L3 ANSWER 2 OF 30 HCAPLUS COPYRIGHT 2004 ACS

ED Entered STN: 25 Jul 2003

ACCESSION NUMBER: 2003:570644 HCAPLUS

DOCUMENT NUMBER: 139:133575

TITLE: Preparation of bicyclic pyrimidinyl derivatives as adenosine receptor ligands

INVENTOR(S): Castelhana, Arlindo L.; McKibben, Bryan

PATENT ASSIGNEE(S): OSI Pharmaceuticals Inc., USA

SOURCE: U.S. Pat. Appl. Publ., 105 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

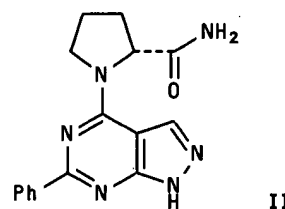
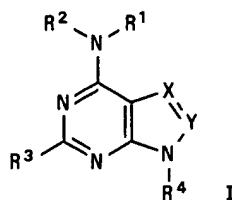
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003139427	A1	20030724	US 2002-227378	20020823
PRIORITY APPLN. INFO.:			US 2002-227378	20020823

OTHER SOURCE(S): MARPAT 139:133575

GI



AB Title compds. I [Y = N, CR⁵ and X = N, CR⁶ wherein X, Y are both N or when Y = CR⁵, X = N or when X = CR⁶, Y = N; R¹⁻² = H, alkoxy, aminoalkyl, etc; R³⁻⁴ = H, alkyl, aryl, alkylaryl] are prepd. For instance, 3-amino-4-carbamoylpyrazole is acylated with benzoyl chloride (Pyridine, 50°, 5-6 h), cyclized to the corresponding pyrazolopyrimidine (water, K₂CO₃, 100°, 16 h), converted to the chloride (POCl₃, 106°, 2 h) and used for reactions with various amines to give the example compds., e.g., II. II has K_i = 76.7 nM for the adenosine A1 receptor, K_i = 242.7 nM for A2a and K_i = 1480.5 nM for A2b. I are useful for the treatment of.

IT	***246855-41-4P***	***246855-42-5P***	***251945-90-1P***
	251945-91-2P	***251945-92-3P***	***251945-93-4P***
	251945-94-5P	***251945-95-6P***	***251945-96-7P***

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L3 ANSWER 2 OF 30 HCAPLUS COPYRIGHT 2004 ACS

251945-97-8P	***251945-98-9P***	***251945-99-0P***
251946-00-6P	***251946-01-7P***	***251946-03-9P***
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251946-33-5P	***251946-34-6P***	***251946-35-7P***
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343632-21-3P	***343632-31-5P***	***343632-32-6P***
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343632-37-1P	***343632-38-2P***	***343632-50-8P***
343969-79-9P	***343969-97-1P***	***443118-43-2P***
443118-44-3P	***443118-78-3P***	***443760-82-5P***
565234-92-6P		

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of bicyclic pyrazolo- imidazo- and triazolopyrimidinyl derivs. as adenosine receptor ligands)

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L3 ANSWER 3 OF 30 HCAPLUS COPYRIGHT 2004 ACS

ED Entered STN: 04 Jul 2003

ACCESSION NUMBER: 2003:511094 HCAPLUS

DOCUMENT NUMBER: 139:85365

TITLE: Preparation of pyrrolopyrimidine A_{2b} selective antagonist compounds,
method of synthesis and therapeutic use

INVENTOR(S): Castelhana, Arlindo L.; Mckibben, Bryan; Steinig, Arno G.

PATENT ASSIGNEE(S): Osi Pharmaceuticals, Inc., USA

SOURCE: PCT Int. Appl., 223 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003053361	A2	20030703	WO 2002-US40890	20021220
WO 2003053361	A3	20031224		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR,
CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID,
IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD,
MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG,
SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW,
AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY,
CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK,
TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

US 2003229067	A1	20031211	US 2002-326005	20021220
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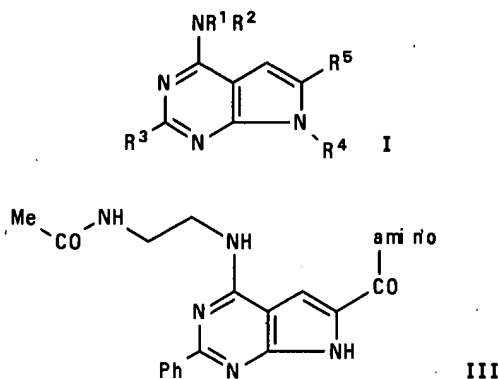
PRIORITY APPLN. INFO.:

US 2001-343443 P 20011220

OTHER SOURCE(S): CASREACT 139:85365; MARPAT 139:85365

GI

L3 ANSWER 3 OF 30 HCAPLUS COPYRIGHT 2004 ACS



AB The subject invention provides pyrrolopyrimidines (shown as I; see below for variable definitions; e.g.

N-[2-[6-[1-[2-(2-chlorophenyl)ethyl]piperidin-4-yloxymethyl]-2-phenyl-7H-pyrrolo[2,3-d]pyrimidin-4-yl-amino]ethyl]acetamide (II)) or a specific enantiomer thereof, or a specific tautomer thereof, or a pharmaceutically acceptable salt thereof, and a method for treating a disease assocd. with the A_{2b} adenosine receptor. For I: R¹ is a (un)substituted alkyl (substituent = hydroxyl, dihydroxy, carboxyl, -C(O)NR^aR^b, -NR^aR^b, -NR^aC(O)NR^aR^b, -NR^aC(O)OR^a, -OC(O)NR^aR^b, or -NHC(O)R^a). R² is H or a (un)substituted alkyl (substituent = hydroxyl, dihydroxy, carboxyl, -C(O)NR^aR^b, -NR^aR^b, -NR^aC(O)NR^aR^b, -NR^aC(O)OR^a, -OC(O)NR^aR^b, or -NHC(O)R^a), or R¹, R² and N together form a substituted piperazine, substituted azetidine, or a pyrrolidine ring substituted with -(CH₂)₂OH or -CH₂C(O)OH. R³ is a (un)substituted Ph or a 5-6 membered heteroaryl ring, wherein the substituent is halogen, hydroxyl, cyano, (C₁-C₁₅)alkyl, (C₁-C₁₅)alkoxyl or -NR^aR^b; R⁴ is H or (un)substituted (C₁-C₁₅)alkyl; R⁵ is -(CH₂)_mOR⁶, -CHNOR⁷, -C(O)NR⁸R⁹, -(CH₂)_mC(O)OR¹⁰, -(CH₂)_kC(O)NR¹¹R¹²; addnl. details are given in the claims. Radioligand binding assays yielded selectivities for the A_{2b} receptor relative to the A₁, A_{2a} and A₃ receptors for 9 examples of I, e.g. 26 times for II. About 26 example preps. of I and intermediates and characterization data for hundreds of I and intermediates are included. For example, III can be prepd. by reacting 4-chloro-2-phenyl-7H-pyrrolo[2,3-d]pyrimidine with PhSO₂Cl and a reducing agent in the presence of solvent to produce 7-benzenesulfonyl-4-chloro-2-phenyl-7H-pyrrolo[2,3-d]pyrimidine, which was reacted with CO₂ in the presence of LDA and a solvent to produce lithium 7-benzenesulfonyl-4-chloro-2-phenyl-7H-pyrrolo[2,3-d]pyrimidine-6-carboxylate, which was reacted with AcNHCH₂CH₂NH₂ in the presence of solvent to give 4-(2-acetylaminoethylamino)-7-benzenesulfonyl-2-phenyl-7H-pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, which was deprotected with a hydroxide base and subsequently condensed with amines.

IT ***553634-53-0P***

N-[2-[[6-Methyl-7-[2-oxo-2-[4-(3-phenylallyl)piperazin-1-yl]ethyl]-2-phenyl-7H-pyrrolo[2,3-d]pyrimi-

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din-4-yl]amino]ethyl]acetamide

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; prepn. of pyrrolopyrimidine A_{2b} selective antagonist compds., method of synthesis and therapeutic use)

L3 ANSWER 4 OF 30 HCAPLUS COPYRIGHT 2004 ACS

ED Entered STN: 13 Jun 2003

ACCESSION NUMBER: 2003:454286 HCAPLUS

DOCUMENT NUMBER: 139:36534

TITLE: Preparation of arylpyrrolopyrimidines as adenosine A₁ and A₃ receptor inhibitors

INVENTOR(S): Castelhana, Arlindo L.; McKibben, Bryan; Werner, Douglas S.; Witter, David

PATENT ASSIGNEE(S): OSI Pharmaceuticals, Inc., USA

SOURCE: PCT Int. Appl., 170 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003048120	A2	20030612	WO 2002-US38055	20021127
WO 2003048120	A3	20030904		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

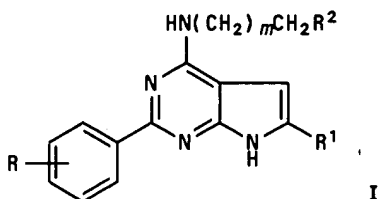
PRIORITY APPLN. INFO.:

US 2001-335273P P 20011130

US 2001-337274P P 20011130

OTHER SOURCE(S): MARPAT 139:36534

L3 ANSWER 4 OF 30 HCAPLUS COPYRIGHT 2004 ACS
GI



AB Arylpyrrolopyrimidines I [$m = 0-3$; $R =$ halogen, alkyl, alkoxy, OH, NH_2 , alkylamino; $R^1 =$ H, (un)substituted alkyl, aryl, aralkyl; $R^2 =$ (un)substituted imidazole, pyrazole, attached through C] which specifically inhibit the adenosine A_1 and A_3 receptors were prepd. Thus, 4-chloro-2-phenyl-7H-pyrrolo[2,3-d]pyrimidine was treated with histamine to give the 4-[2-(1H-imidazol-2-yl)ethyl]amino analog which had A_3 inhibiting activity ≥ 10 times greater than that of ref. compds.

IT ***541503-67-7P*** ***541503-83-7P*** ***541503-85-9P***
541503-91-7P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of arylpyrrolopyrimidines as adenosine A_1 and A_3 receptor inhibitors)

IT ***251946-11-9P*** ***251947-22-5P*** ***251947-24-7P***
343632-31-5P ***343632-32-6P*** ***343632-33-7P***
343632-35-9P ***343632-36-0P*** ***343632-37-1P***
343632-38-2P ***343632-50-8P*** ***443118-47-6P***
541503-35-9P ***541503-69-9P*** ***541503-71-3P***
541503-73-5P ***541503-75-7P*** ***541503-77-9P***
541503-80-4P ***541503-87-1P***

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of arylpyrrolopyrimidines as adenosine A_1 and A_3 receptor inhibitors)

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L3 ANSWER 5 OF 30 HCAPLUS COPYRIGHT 2004 ACS

ED Entered STN: 18 Apr 2003

ACCESSION NUMBER: 2003:300617 HCAPLUS

DOCUMENT NUMBER: 138:321287

TITLE: Preparation of deazapurines as adenosine A₃ receptor antagonists.

INVENTOR(S): Castelhana, Arlindo L.; McKibben, Bryan; Witter, David J.

PATENT ASSIGNEE(S): OSI Pharmaceuticals, Inc., USA

SOURCE: U.S. Pat. Appl. Publ., 77 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

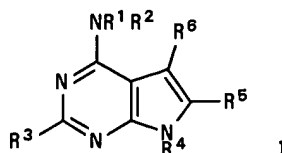
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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US 2003073708	A1	20030417	US 2001-6405	20011130
US 6673802	B2	20040106		

PRIORITY APPLN. INFO.:

US 2000-250748P P 20001201

OTHER SOURCE(S): MARPAT 138:321287

GI



AB Title compds. [I; R¹, R² = H, (substituted) alkyl, aryl, aralkyl; R¹R² = atoms to form (substituted) heterocyclyl; R³ = (substituted) alkyl, aryl, aralkyl; R⁴ = H, (substituted) alkyl, aryl, aralkyl; R⁵, R⁶ = H, halo, (substituted) alkyl, aryl, alkylaryl; R⁴R⁵ or R⁵R⁶ = (substituted) heterocyclyl, carbocyclyl], were prepd. Thus, 2-phenyl-7H-pyrrolo[2,3-d]pyrimidin-4-ylamine and histamine were heated at 120° in Me₂SO for 6.5 h to give 43% [2-(3H-imidazol-4-yl)ethyl] [2-phenyl-7H-pyrrolo[2,3-d]pyrimidin-4-yl]amine. The latter had 10 times the A₃ receptor binding affinity of a ref. compd.

IT ***443118-47-6P***

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(claimed compd.; prepn. of deazapurines as adenosine A₃ receptor antagonists)

IT ***246855-41-4P*** ***246855-42-5P*** ***251945-90-1P***

251945-91-2P ***251945-92-3P*** ***251945-93-4P***

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251945-94-5P	***251945-95-6P***	***251945-96-7P***
251945-97-8P	***251945-98-9P***	***251945-99-0P***
251946-00-6P	***251946-01-7P***	***251946-04-0P***
251946-05-1P	***251946-06-2P***	***251946-07-3P***
251946-08-4P	***251946-09-5P***	***251946-10-8P***
251946-11-9P	***251946-12-0P***	***251946-13-1P***
251946-14-2P	***251946-15-3P***	***251946-16-4P***
251946-17-5P	***251946-18-6P***	***251946-19-7P***
251946-20-0P	***251946-21-1P***	***251946-22-2P***
251946-23-3P	***251946-24-4P***	***251946-25-5P***
251946-26-6P	***251946-27-7P***	***251946-28-8P***
251946-29-9P	***251946-30-2P***	***251946-31-3P***
251946-32-4P	***251946-33-5P***	***251946-34-6P***
251946-35-7P	***251946-36-8P***	***251946-37-9P***
251946-38-0P	***251946-39-1P***	***251946-40-4P***
251946-41-5P	***251946-42-6P***	***251946-43-7P***
251946-44-8P	***251946-45-9P***	***251946-46-0P***
251946-47-1P	***251946-48-2P***	***251946-54-0P***
251946-55-1P	***251946-56-2P***	***251946-57-3P***
251946-58-4P	***251946-59-5P***	***343632-17-7P***
343632-31-5P	***343632-32-6P***	***343632-35-9P***
343632-37-1P	***343632-38-2P***	***343632-50-8P***
500736-03-8P	***512848-47-4P***	***512848-48-5P***

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of deazapurines as adenosine A₃ receptor antagonists)

IT ***343631-96-9***

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of deazapurines as adenosine A₃ receptor antagonists)

IT ***251947-22-5P*** ***251947-24-7P***

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of deazapurines as adenosine A₃ receptor antagonists)

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L3 ANSWER 6 OF 30 HCAPLUS COPYRIGHT 2004 ACS

ED Entered STN: 07 Mar 2003

ACCESSION NUMBER: 2003:174478 HCAPLUS

DOCUMENT NUMBER: 138:221598

TITLE: Preparation of pyrrolo[2,3-d]pyrimidinamines as selective adenosine A₁ receptor inhibitors for treatment of asthma, COPD, and other conditions

INVENTOR(S): Castelhana, Arlindo L.; McKibben, Bryan; Witter, David J.

PATENT ASSIGNEE(S): OSI Pharmaceuticals, Inc., USA

SOURCE: U.S. Pat. Appl. Publ., 79 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

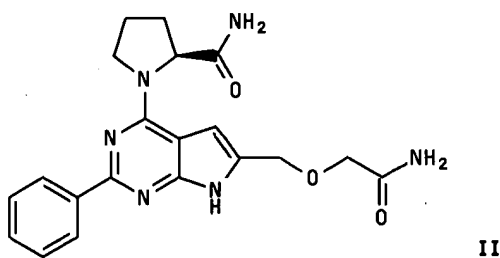
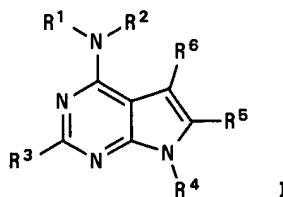
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003045536	A1	20030306	US 2001-280	20011130
US 6680324	B2	20040120		

PRIORITY APPLN. INFO.:

US 2000-250895P P 20001201

OTHER SOURCE(S): MARPAT 138:221598

GI



AB Title diazapurinamines I [wherein R¹, R², and R⁴ = independently H or (un)substituted alkyl(aryl) or aryl; or NR¹R² = (un)substituted heterocyclyl; R³ = (un)substituted alkyl(aryl), aryl,

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CO₂H, carboxy esters, or carboxamides; or C₂R³R⁴ or C₂R⁵R⁶ = (un)substituted carbocyclyl or heterocyclyl; R⁵ and R⁶ = independently H, halo, or (un)substituted alkyl(aryl) or aryl; and pharmaceutically acceptable salts and prodrugs thereof] were prep'd. as adenosine A₁ specific inhibitors. For example, 4-chloro-5-methyl-2-phenyl-1H-pyrrolo[2,3-*d*]pyrimidine was protected with di-*t*-Bu dicarbonate (80%), brominated (84%), coupled with anhyd. Me glycolate (99%), coupled with L-prolinamide (92%), and deprotected (93%) to give II. The latter exhibited adenosine A₁ receptor binding equal to or surpassing that of ref. compds. and is expected to have better water soly. (cLogP = 1.5) than ref. compds. (cLogP = 3.8). Efficacy and structure activity profiles of diazapurines of the invention are also disclosed. Thus, I are useful for the treatment of asthma, chronic obstructive pulmonary disease (COPD), allergic rhinitis, upper respiratory disorder, and congestive heart failure (no data).

IT ***246855-41-4P***

4-[(4-*trans*-Hydroxycyclohexyl)amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

251946-08-4P ***251946-14-2P***

4-[(3-*tert*-Butyloxy-3-oxopropyl)amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine***251946-15-3P*** 4-[(2-Hydroxyethyl)amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine
251946-18-6P4-[(4-*cis*-Benzoyloxycyclohexyl)amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

251946-24-4P

4-[(3-Hydroxy-3-oxopropyl)amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine***251946-31-3P*** 4-[(2-Aminoethyl)amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine
251946-42-6P4-[[1-Methyl-2-[[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(A₁ receptor inhibitor; prepn. of pyrrolopyrimidinamines adenosine A₁ receptor inhibitors from aminocyanopyrroles for treatment of asthma, COPD, and other conditions)

IT ***246855-42-5P***

4-[(2-Acetylaminoethyl)amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

251945-90-1P

4-[(4-*trans*-Hydroxycyclohexyl)amino]-6-methyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

251945-91-2P

4-[(4-*trans*-Hydroxycyclohexyl)amino]-5-methyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine***251945-92-3P*** 4-[(4-*trans*-Hydroxycyclohexyl)amino]-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine
251945-93-4P4-[(4-*trans*-Hydroxycyclohexyl)amino]-5,6-dimethyl-2-(3-pyridyl)-7H-pyrrolo[2,3-*d*]pyrimidine

251945-94-5P

4-[(4-*trans*-Hydroxycyclohexyl)amino]-5,6-dimethyl-2-(2-furyl)-7H-pyrrolo[2,3-*d*]pyrimidine

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251945-95-6P

4-[(4-*trans*-Hydroxycyclohexyl)amino]-5,6-dimethyl-2-(3-furyl)-7*H*-pyrrolo[2,3-*d*]pyrimidine

251945-96-7P

4-[(4-*trans*-Hydroxycyclohexyl)amino]-5,6-dimethyl-2-cyclopentyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

251945-97-8P

4-[(4-*trans*-Hydroxycyclohexyl)amino]-5,6-dimethyl-2-(2-thienyl)-7*H*-pyrrolo[2,3-*d*]pyrimidine

251945-98-9P

4-[(4-*trans*-Hydroxycyclohexyl)amino]-5,6-dimethyl-2-(3-thienyl)-7*H*-pyrrolo[2,3-*d*]pyrimidine

251945-99-0P

4-[(4-*trans*-Hydroxycyclohexyl)amino]-5,6-dimethyl-2-(4-fluorophenyl)-7*H*-pyrrolo[2,3-*d*]pyrimidine

251946-00-6P

4-[(4-*trans*-Hydroxycyclohexyl)amino]-5,6-dimethyl-2-(3-fluorophenyl)-7*H*-pyrrolo[2,3-*d*]pyrimidine

251946-01-7P

4-[(4-*trans*-Hydroxycyclohexyl)amino]-5,6-dimethyl-2-(2-fluorophenyl)-7*H*-pyrrolo[2,3-*d*]pyrimidine

251946-03-9P

251946-06-2P

4-[(2-*trans*-Hydroxycyclopentyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

251946-07-3P

4-[(3-*trans*-Hydroxycyclopentyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

251946-10-8P

4-[(3-Amino-3-oxopropyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

251946-11-9P

4-[(3-(Cyclopropylmethylamino)-3-oxopropyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

251946-12-0P

4-[(2-Amino-2-oxoethyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

251946-13-1P

4-[(2-(Methylamino)-2-oxoethyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

251946-16-4P

4-[(3-Hydroxypropyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

251946-17-5P

4-[(4-Hydroxybutyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

251946-19-7P

4-[(3-Cyclohexenyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

251946-20-0P

4-[(4-*cis*-Hydroxycyclohexyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

251946-21-1P

4-[(3-(Dimethylamino)-3-oxopropyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

251946-22-2P

4-[(2-Formylaminoethyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

251946-23-3P

4-[(3-Acetylaminopropyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

251946-25-5P

4-[(3-Aminopropyl)amino]-5,6-dimethyl-2-phenyl-7*H*-pyrrolo[2,3-*d*]pyrimidine

251946-26-6P

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4-[[3-(Methylamino)-3-oxopropyl]amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

251946-27-7P

4-[[2-[(Cyclopropanecarbonyl)amino]ethyl]amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

251946-28-8P

4-[(2-Isobutyrylaminoethyl)amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

251946-29-9P

4-[(3-Propionylaminopropyl)amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

251946-30-2P

4-[[2-(Methylsulfonylamino)ethyl]amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

251946-32-4P

4-[(2-Propionylaminoethyl)amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

251946-33-5P

4-[[2-(*N*'-Methylureido)ethyl]amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

251946-34-6P

4-[[2-(*N*'-Ethylureido)ethyl]amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

251946-35-7P

4-[(2-Pyruvylamidoethyl)amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine***251946-36-8P*** 4-[(2-Ureidoethyl)amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

251946-37-9P

4-[(2-Acetylaminopropyl)amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

251946-38-0P

(R)-4-[(2-Acetylaminopropyl)amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

251946-39-1P

(R)-4-[(1-Methyl-2-acetylaminooethyl)amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

251946-40-4P

(S)-4-[(2-Acetylaminopropyl)amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

251946-41-5P

(S)-4-[(1-Methyl-2-acetylaminooethyl)amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

251946-44-8P

(S,S)-4-[(2-Acetylaminocyclohexyl)amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

251946-45-9P

4-[(2-Methyl-2-acetylaminopropyl)amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

251946-46-0P

4-[(1-Methyl-2-acetylaminooethyl)amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

251946-47-1P

(R,R)-4-[(2-Acetylaminocyclohexyl)amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

251946-48-2P

4-[(2-Acetyloxyethyl)amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

251946-49-3P

251946-50-6P

251946-54-0P

4-[[2-(*N*'-Methylureido)propyl]amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

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251946-55-1P

4-[(2-Acetamidobutyl)amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

251946-56-2P

4-[[2-(*N'*-Methylureido)butyl]amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

251946-57-3P

4-[(*trans*-4-Hydroxycyclohexyl)amino]-2-(3-chlorophenyl)-7H-pyrrolo[2,3-*d*]pyrimidine

251946-58-4P

4-[(*trans*-4-Hydroxycyclohexyl)amino]-2-(3-fluorophenyl)-7H-pyrrolo[2,3-*d*]pyrimidine

251946-59-5P

251947-22-5P

251947-24-7P

343632-03-1P

343632-04-2P

343632-05-3P

343632-07-5P

343632-08-6P

343632-09-7P

343632-10-0P

343632-11-1P

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343632-15-5P

343632-16-6P

343632-17-7P

343632-19-9P

343632-20-2P

343632-21-3P

343969-79-9P

343969-97-1P

443118-43-2P

443118-78-3P

443760-82-5P

500736-02-7P

4-[[2-Methyl-1-[(1,1-dimethylethoxy)carbonyl]amino]ethyl]amino]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-*d*]pyrimidine

500736-03-8P

500736-09-4P

500736-10-7P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(A₁ receptor inhibitor; prepn. of pyrrolopyrimidinamines adenosine A₁ receptor inhibitors from aminocyanopyrroles for treatment of asthma, COPD, and other conditions)

IT ***343632-97-3P***

443760-84-7P

443760-85-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; prepn. of pyrrolopyrimidinamines adenosine A₁ receptor inhibitors from aminocyanopyrroles for treatment of asthma, COPD, and other conditions)

L3 ANSWER 7 OF 30 HCAPLUS COPYRIGHT 2004 ACS

ED Entered STN: 24 Sep 2002

ACCESSION NUMBER: 2002:720128 HCAPLUS

DOCUMENT NUMBER: 137:379680

TITLE: Synthesis, Molecular Modeling Studies, and Pharmacological Activity of Selective A₁ Receptor Antagonists

AUTHOR(S): Bondavalli, Francesco; Botta, Maurizio; Bruno, Olga; Ciacci, Andrea; Corelli, Federico; Fossa, Paola; Lucacchini, Antonio; Manetti, Fabrizio; Martini, Claudia; Menozzi, Giulia; Mosti, Luisa; Ranise, Angelo; Schenone, Silvia; Tafi, Andrea; Trincavelli, Maria Letizia

CORPORATE SOURCE: Dipartimento di Scienze Farmaceutiche, Universita degli Studi di Genova, Genoa, I-16132, Italy

SOURCE: Journal of Medicinal Chemistry (2002), 45(22), 4875-4887
CODEN: JMCMAR; ISSN:0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB We present a combined computational study aimed at identifying the three-dimensional structural properties required for different classes of compds. to show antagonistic activity toward the A₁ adenosine receptor (AR). Particularly, an approach combining pharmacophore mapping, mol. alignment, and pseudoreceptor generation was applied to derive a hypothesis of the interaction pathway between a set of A₁ AR antagonists taken from the literature and a model of the putative A₁ receptor. The pharmacophore model consists of seven features and represents an improvement of the N⁶-C⁸ model, generally reported as the most probable pharmacophore model for A₁ AR agonists and antagonists. It was used to build up a pseudoreceptor model able to rationalize the relationships between structural properties and biol. data of, and external to, the training set. In fact, to further assess its statistical significance and predictive power, the pseudoreceptor was employed to predict the free energy of binding assocd. with compds. constituting a test set. While part of these mols. was also taken from the literature, the remaining compds. were designed and synthesized by our research group. All of the new compds. were tested for their affinity toward A₁, A_{2a}, and A₃ AR, showing interesting antagonistic activity and A₁ selectivity.

IT ***476006-54-9***

RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(synthesis, mol. modeling studies, and pharmacol. activity of selective A₁ receptor antagonists)

REFERENCE COUNT: 70 THERE ARE 70 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L3 ANSWER 8 OF 30 HCAPLUS COPYRIGHT 2004 ACS

ED Entered STN: 26 Jul 2002

ACCESSION NUMBER: 2002:555495 HCAPLUS

DOCUMENT NUMBER: 137:109485

TITLE: Preparation of pyrrolopyrimidinylprolineamides and analogs as adenosine receptor antagonists

INVENTOR(S): Castelhana, Arlindo L.; McKibben, Bryan; Witter, David J.

PATENT ASSIGNEE(S): Osi Pharmaceuticals, Inc., USA

SOURCE: PCT Int. Appl., 320 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

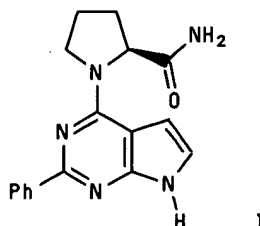
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2002057267	A1	20020725	WO 2001-US45280	20011130
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2002058667	A1	20020516	US 2000-728316	20001201
US 6680322	B2	20040120		
US 2002094974	A1	20020718	US 2000-728616	20001201
US 2003036545	A1	20030220	US 2000-728607	20001201
US 6664252	B2	20031216		
EP 1347980	A1	20031001	EP 2001-997029	20011130
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
NO 2003002482	A	20030728	NO 2003-2482	20030602
PRIORITY APPLN. INFO.:				
			US 1999-169037P P	19991202
			US 2000-728316 A	20001201
			US 2000-728616 A	20001201
			US 2000-728607 A	20001204
			US 1999-168803P P	19991202
			US 1999-169036P P	19991202

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WO 2001-US45280 W 20011130

OTHER SOURCE(S): MARPAT 137:109485

GI



AB Title compds., e.g., I, were prepd. Data for biol. activity of title compds. were given.

IT ***251946-19-7P***

RL: BYP (Byproduct); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of pyrrolopyrimidinylprolineamides and analogs as adenosine receptor antagonists)

IT	***246855-41-4P***	***246855-42-5P***	***251945-90-1P***
	251945-91-2P	***251945-92-3P***	***251945-93-4P***
	251945-94-5P	***251945-95-6P***	***251945-96-7P***
	251945-97-8P	***251945-98-9P***	***251945-99-0P***
	251946-00-6P	***251946-01-7P***	***251946-06-2P***
	251946-07-3P	***251946-08-4P***	***251946-10-8P***
	251946-11-9P	***251946-12-0P***	***251946-13-1P***
	251946-14-2P	***251946-15-3P***	***251946-16-4P***
	251946-17-5P	***251946-18-6P***	***251946-20-0P***
	251946-21-1P	***251946-22-2P***	***251946-23-3P***
	251946-24-4P	***251946-25-5P***	***251946-26-6P***
	251946-27-7P	***251946-28-8P***	***251946-29-9P***
	251946-30-2P	***251946-31-3P***	***251946-32-4P***
	251946-33-5P	***251946-34-6P***	***251946-35-7P***
	251946-36-8P	***251946-37-9P***	***251946-38-0P***
	251946-39-1P	***251946-40-4P***	***251946-41-5P***
	251946-42-6P	***251946-43-7P***	***251946-44-8P***
	251946-45-9P	***251946-46-0P***	***251946-47-1P***
	251946-48-2P	***251946-49-3P***	***251946-50-6P***
	251946-52-8P	***251946-54-0P***	***251946-55-1P***
	251946-56-2P	***251946-57-3P***	***251946-58-4P***
	251946-59-5P	***251947-22-5P***	***251947-24-7P***

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343632-03-1P	***343632-05-3P***	***343632-06-4P***
343632-07-5P	***343632-08-6P***	***343632-09-7P***
343632-10-0P	***343632-11-1P***	***343632-12-2P***
343632-13-3P	***343632-14-4P***	***343632-16-6P***
343632-17-7P	***343632-19-9P***	***343632-20-2P***
343632-21-3P	***343632-31-5P***	***343632-35-9P***
343632-37-1P	***343632-38-2P***	***343632-50-8P***
343969-79-9P	***343969-97-1P***	***443118-47-6P***
443760-78-9P	***443760-79-0P***	***443760-80-3P***
443760-82-5P		

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of pyrrolopyrimidinylprolineamides and analogs as adenosine receptor antagonists)

IT ***443760-84-7P*** ***443760-85-8P***

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of pyrrolopyrimidinylprolineamides and analogs as adenosine receptor antagonists)

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L3 ANSWER 9 OF 30 HCAPLUS COPYRIGHT 2004 ACS

ED Entered STN: 19 Jul 2002

ACCESSION NUMBER: 2002:540257 HCAPLUS

DOCUMENT NUMBER: 137:109288

TITLE: Preparation of pyrrolo[2,3-d]pyrimidines as selective inhibitors of the adenosine A₃ receptor

INVENTOR(S): Castelhana, Arlindo L.; McKibben, Bryan; Witter, David J.

PATENT ASSIGNEE(S): USA

SOURCE: U.S. Pat. Appl. Publ., 83 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

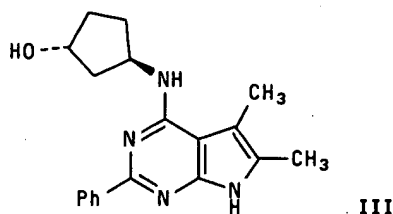
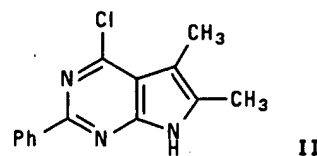
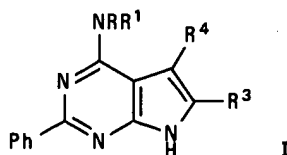
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002094974	A1	20020718	US 2000-728616	20001201
WO 2002057267	A1	20020725	WO 2001-US45280	20011130
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1347980	A1	20031001	EP 2001-997029	20011130
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
NO 2003002482	A	20030728	NO 2003-2482	20030602
PRIORITY APPLN. INFO.:				
			US 1999-169036P P	19991202
			US 1999-169037P P	19991202
			US 2000-728316 A	20001201
			US 2000-728616 A	20001201
			US 2000-728607 A	20001204
			WO 2001-US45280 W	20011130

OTHER SOURCE(S): MARPAT 137:109288

GI

L3 ANSWER 9 OF 30 HCAPLUS COPYRIGHT 2004 ACS



AB Pyrrolopyrimidines **I** [$R = 3\text{-hydroxycyclopentylamino}$ ethylamino carbonylamino Pr, N,N -diethylamino carbonylamino Et, thioacetamido Et, 3-amino acetyloxy cyclopentyl, 3-hydroxycyclopentyl, 2-pyrrolyl carbonyl aminoethyl, 2-imidazolinone Et, 1-aminocarbonyl-2-methylpropyl, 1-aminocarbonyl-2-Ph Et, 3-hydroxyazetidino, 2-imidazoleethyl, acetamidoethyl, 1-(*R*)-phenyl-2-hydroxyethyl, N -methylaminocarbonyl pyridyl-2-methyl; $R^1 = H$; $RR^1N = 3\text{-hydroxypyrrolidino}$, 3-methyloxy carbonylmethyl pyrrolidino, 3-aminocarbonylmethyl pyrrolidino, 3-hydroxymethyl piperidino; $R^3, R^4 = H$, (un)substituted alkyl, aryl] are prep'd. as selective inhibitors of adenosine receptors, particularly the adenosine A_3 receptor, for the treatment of diseases such as asthma, diarrhea, chronic obstructive pulmonary disease, allergic rhinitis, or for the treatment of eye damage caused either by disease or injury. Human adenosine receptors are transformed into yeast; the modified yeast are used to assay the invention compds. **I** for their adenosine receptor binding and selectivities. E.g., 1-(1-phenylethyl)-2-amino-3-cyano-4,5-dimethylpyrrole is acylated with PhCOCl to give the benzamide which undergoes cyclocondensation with concd. H_2SO_4 in MeOH to give a pyrrolopyrimidinone; removal of the phenethyl group with polyphosphoric acid and chlorination of the pyrrolopyrimidinone with POCl_3 gives the intermediate chloropyrrolopyrimidine **II**. E.g., addn. of amines such as trans-3-amino-1-cyclopentanol to **II** in DMSO gives aminopyrrolopyrimidines such as **III**. **III** has a K_i for the adenosine A_1 receptor of 29 nM and a K_i for the adenosine A_3 receptor of 3.1 nM while binding to the adenosine A_{2a} and A_{2b} receptors with K_i values of 191 nM and 1143 nM, resp. Formulations of these compds. are claimed (no data). Methods for the prep'n. of **I** from the acylation of aminopyrroles with acyl chlorides followed by cyclocondensation and deprotection, chlorination, and substitution of the chlorine atom with an amine are claimed.

IT ***251946-42-6P*** ***443118-78-3P***

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL

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(Biological study); PREP (Preparation); USES (Uses)

(intermediate; prepn. of pyrrolo[2,3-d]pyrimidines as selective inhibitors of the adenosine A₃ receptor for the treatment of diseases such as diarrhea, allergic rhinitis, and eye damage resulting from injuries or disease)

IT ***343632-97-3P***

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; prepn. of pyrrolo[2,3-d]pyrimidines as selective inhibitors of the adenosine A₃ receptor for the treatment of diseases such as diarrhea, allergic rhinitis, and eye damage resulting from injuries or disease)

IT ***177499-41-1P***	***246855-41-4P***	***246855-42-5P***
246855-44-7P	***246855-45-8P***	***246855-46-9P***
246855-48-1P	***251945-90-1P***	***251945-91-2P***
251945-92-3P	***251945-93-4P***	***251945-94-5P***
251945-95-6P	***251945-96-7P***	***251945-97-8P***
251945-98-9P	***251946-03-9P***	***251946-06-2P***
251946-07-3P	***251946-08-4P***	***251946-10-8P***
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251946-29-9P	***251946-30-2P***	***251946-31-3P***
251946-32-4P	***251946-33-5P***	***251946-34-6P***
251946-35-7P	***251946-36-8P***	***251946-37-9P***
251946-38-0P	***251946-39-1P***	***251946-40-4P***
251946-41-5P	***251946-44-8P***	***251946-45-9P***
251946-46-0P	***251946-47-1P***	***251946-48-2P***
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343632-14-4P	***343632-15-5P***	***343632-17-7P***
343632-31-5P	***343632-32-6P***	***343632-33-7P***
343632-35-9P	***343632-36-0P***	***343632-37-1P***
343632-38-2P	***343632-50-8P***	***343632-77-9P***
343632-78-0P	***343632-79-1P***	***343633-16-9P***
343969-97-1P	***443118-21-6P***	***443118-22-7P***
443118-23-8P	***443118-24-9P***	***443118-26-1P***

L3 ANSWER 9 OF 30 HCAPLUS COPYRIGHT 2004 ACS

443118-36-3P	***443118-41-0P***	***443118-42-1P***
443118-43-2P	***443118-44-3P***	***443118-45-4P***
443118-46-5P	***443118-47-6P***	***443118-48-7P***
443118-49-8P	***443118-50-1P***	***443118-51-2P***
443118-52-3P	***443118-53-4P***	***443118-54-5P***
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443118-70-5P	***443118-71-6P***	***443118-72-7P***
443118-73-8P		

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(invention compd.; prepn. of pyrrolo[2,3-d]pyrimidines as selective inhibitors of the adenosine A₃ receptor for the treatment of diseases such as diarrhea, allergic rhinitis, and eye damage resulting from injuries or disease)

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L3 ANSWER 10 OF 30 HCAPLUS COPYRIGHT 2004 ACS

ED Entered STN: 18 May 2002

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DOCUMENT NUMBER: 136:386128

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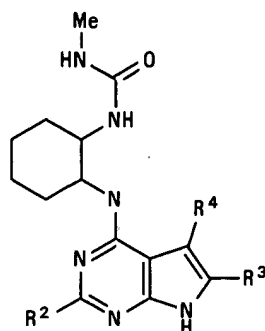
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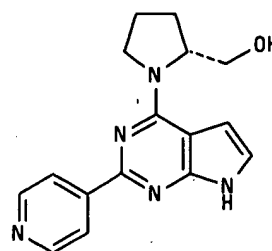
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GI

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I



II

AB Title compds. I and analogs [R^2 = 5-6 membered arom. ring; R^{3-4} = H, alkyl] were prepd. Over 100 examples were provided. Intermediate 4-chloro-7H-pyrrolo[2,3-d]pyrimidines were prepd. by several routes from appropriately substituted cyano-pyrroles. Thus, 4-chloro-2-(4-pyridyl)-7H-pyrrolo[2,3-d]pyrimidine hydrochloride was reacted with D-prolinol (2.3 mol equiv) in DMSO at 120°C for 18 h to yield II in 13% yield after purifn. Compd. I [R^2 = Ph; R^{3-4} = Me] exhibited 10-fold selectivity for binding to the adenosine A_1 receptor than to A_{2a} , A_{2b} or A_3 receptors. ClogP values were detd. for selected example compds. I are useful for the treatment of COPD, allergic rhinitis, etc.

IT ***251946-19-7P***, 1H-Pyrrolo[2,3-d]pyrimidin-4-amine,
N-3-cyclohexen-1-yl-5,6-dimethyl-2-phenyl-

RL: BSU (Biological study, unclassified); BYP (Byproduct); PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(prepn. and use of substituted 7H-pyrrolo[2,3-b]pyrimidines as selective adenosine A_1 , A_{2a} and A_3 receptor antagonists)

IT ***251946-18-6P***, Cyclohexanol,

4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-benzoate (ester), *cis*-

RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(prepn. and use of substituted 7H-pyrrolo[2,3-b]pyrimidines as selective adenosine A_1 , A_{2a} and A_3 receptor antagonists)

IT ***246855-41-4P***, Cyclohexanol,

4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-*trans* ***246855-42-

5P***, Acetamide, N-[2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]ethyl]-

251945-90-1P, Cyclohexanol,

4-[(6-methyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, *trans*- ***251945-91-

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2P*** , Cyclohexanol, 4-[(5-methyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, *trans*-
 251945-92-3P , Cyclohexanol, 4-[(2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, *trans*-
 251945-93-4P , Cyclohexanol,
 4-[[5,6-dimethyl-2-(3-pyridinyl)-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl]amino]-, *trans*-
 251945-94-5P , Cyclohexanol,
 4-[[2-(2-furanyl)-5,6-dimethyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl]amino]-, *trans*-
 251945-95-6P , Cyclohexanol,
 4-[[2-(3-furanyl)-5,6-dimethyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl]amino]-, *trans*-
 251945-96-7P , Cyclohexanol,
 4-[(2-cyclopentyl-5,6-dimethyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, *trans*-
 251945-97-8P , Cyclohexanol,
 4-[[5,6-dimethyl-2-(2-thienyl)-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl]amino]-, *trans*-
 251945-98-9P , Cyclohexanol,
 4-[[5,6-dimethyl-2-(3-thienyl)-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl]amino]-, *trans*-
 251945-99-0P , Cyclohexanol,
 4-[[2-(4-fluorophenyl)-5,6-dimethyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl]amino]-, *trans*-
 251946-00-6P , Cyclohexanol,
 4-[[2-(3-fluorophenyl)-5,6-dimethyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl]amino]-, *trans*-
 251946-01-7P , Cyclohexanol,
 4-[[2-(2-fluorophenyl)-5,6-dimethyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl]amino]-, *trans*-
 251946-03-9P , Cyclohexanol,
 2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, (1*R*,2*R*)-*rel*
 251946-04-0P , 1,2-Cyclohexanediol,
 4-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, (1*R*,2*R*)-*rel*
 251946-05-1P , 1,2-Cyclohexanediol,
 4-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, (1*R*,2*S*)-*rel*
 251946-06-2P , Cyclopentanol,
 2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, (1*R*,2*R*)-*rel*
 251946-07-3P , Cyclopentanol,
 3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, (1*R*,3*R*)-*rel*
 251946-08-4P , Cyclopentanol,
 3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, (1*R*,3*S*)-*rel*
 251946-09-5P , Propanamide,
 3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, ***251946-11-9P***,
 Propanamide, *N*-(cyclopropylmethyl)-3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-
 251946-12-0P , Acetamide,
 2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, ***251946-13-1P***, Acetamide,
 2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-*N*-methyl-
 251946-14-2P , β -Alanine, *N*-(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)-,
 1,1-dimethylethyl ester ***251946-15-3P*** , Ethanol,

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2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]- ***251946-16-4P***, 1-Propanol,
 3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]- ***251946-17-5P***, 1-Butanol,
 4-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]- ***251946-20-0P***,
 Cyclohexanol, 4-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, *cis*
 251946-21-1P, Propanamide,
 3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-*N,N*-dimethyl-
 251946-22-2P, Formamide,
N-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]- ***251946-
 23-3P***, Acetamide,
N-[3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]propyl]-
 251946-24-4P, β -Alanine, *N*-(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)-
 251946-25-5P, 1,3-Propanediamine,
N-(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)- ***251946-26-6P***, Propanamide,
 3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-*N*-methyl-
 251946-27-7P, Cyclopropanecarboxamide,
N-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]- ***251946-
 28-8P***, Propanamide,
N-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]-2-methyl-,
 251946-29-9P, Propanamide,
N-[3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]propyl]-
 251946-30-2P, Methanesulfonamide,
N-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]- ***251946-
 31-3P***, 1,2-Ethanediamine, *N*-(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)-
 251946-32-4P, Propanamide,
N-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]- ***251946-
 33-5P***, Urea,
N-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]-*N'*-methyl-
 251946-34-6P, Urea,
N-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]-*N'*-ethyl-
 251946-35-7P, Propanamide,
N-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]-2-oxo-
 251946-36-8P, Urea,
 [2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]- ***251946-37-
 9P***, Acetamide,
N-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-1-methylethyl]-
 251946-38-0P, Acetamide,
N-[(1*R*)-2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-1-methylethyl]-
 251946-39-1P, Acetamide,
N-[(2*R*)-2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]propyl]-
 251946-40-4P, Acetamide,

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N-[(1*S*)-2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-1-methylethyl]-
251946-41-5P , Acetamide,

N-[(2*S*)-2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]propyl]-
251946-42-6P , Carbamic acid,

[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]propyl]-, 1,1-dimethylethyl ester
251946-43-7P , Carbamic acid,

[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-1-methylethyl]-, 1,1-dimethylethyl
ester ***251946-44-8P*** , Acetamide,

N-[(1*S*,2*S*)-2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]cyclohexyl]-
251946-45-9P , Acetamide,

N-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-1,1-dimethylethyl]-
251946-46-0P , Acetamide,

N-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]propyl]-
251946-47-1P , Acetamide,

N-[(1*R*,2*R*)-2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]cyclohexyl]-
251946-48-2P , Ethanol,

2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, acetate (ester)
251946-49-3P , Propanamide,

3-amino-*N*-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]-
251946-50-6P , Butanoic acid,

4-[[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]amino]-4-oxo-
251946-52-8P , Glycine,

(1*R*,3*S*)-3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]cyclopentyl ester, *rel*-,
mono(trifluoroacetate) ***251946-54-0P*** , Urea,

N-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-1-methylethyl]-*N*'-methyl-
251946-55-1P , Acetamide,

N-[1-[[[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]methyl]propyl]-
251946-56-2P , Urea,

N-[1-[[[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]methyl]propyl]-*N*'-methyl-
251946-57-3P , Cyclohexanol,

4-[[2-(3-chlorophenyl)-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl]amino]-, *trans*- ***251946-58-
4P*** , Cyclohexanol, 4-[[2-(3-fluorophenyl)-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl]amino]-, *trans*-

251946-59-5P , Cyclohexanol,

4-[[2-(4-pyridinyl)-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl]amino]-, *trans*- ***251947-22-
5P*** , Acetamide,

N-[*trans*-4-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]cyclohexyl]-
251947-24-7P , Methanesulfonamide,

N-[*trans*-4-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]cyclohexyl]-
343631-95-8P , Propanamide,

N-[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]-2,2-dimethyl-

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343631-96-9P , 1,2-Cyclohexanediamine,
N-(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)-, (1R,2R)- ***343631-97-
0P*** , Propanamide,
3-[[2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]ethyl]amino]-
343631-99-2P , Acetamide,
2-(cyclopropylamino)-N-[2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]ethyl]-
343632-03-1P , 1,2-Cyclohexanediol,
4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, (1R,2S,4R)-rel
343632-04-2P , Cyclohexanol,
4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, benzoate (ester)
343632-05-3P , Cyclohexanol,
4-[(5,6,7-trimethyl-2-phenyl-7H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]-, trans-
343632-06-4P , Cyclohexanol,
4-[[2-(3-furanyl)-5,6-dimethyl-7-(1-phenylethyl)-7H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans-
343632-07-5P , Cyclohexanol,
4-[[5,6-dimethyl-2-phenyl-7-(1-phenylethyl)-7H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]-, trans-
343632-08-6P , 7H-Pyrrolo[2,3-d]pyrimidin-4-amine,
5,6-dimethyl-2-phenyl-7-(1-phenylethyl)-N-(3-pyridinylmethyl)- ***343632-09-7P*** ,
Acetamide,
N-[2-[[5,6-dimethyl-2-phenyl-7-(1-phenylethyl)-7H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]ethyl]-
343632-10-0P , 7H-Pyrrolo[2,3-d]pyrimidin-4-amine,
5,6-dimethyl-N-(2-methylpropyl)-2-phenyl-7-(1-phenylethyl)- ***343632-11-1P*** , Propanamide,
N-[3-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]propyl]-2-methyl-
343632-12-2P , Urea,
N-[3-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]propyl]-N'-methyl-
343632-13-3P , Acetamide,
N-[4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]butyl]- ***343632-
14-4P*** , Urea,
N-[4-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]butyl]-N'-methyl-
343632-15-5P , Cyclopropanecarboxamide,
1-amino-N-[2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]ethyl]-
343632-16-6P , Propanamide,
3-amino-N-[3-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]propyl]-
343632-17-7P , Acetamide,
2-amino-N-[3-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]propyl]-
343632-19-9P , Urea,
N-[2-[(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]cyclohexyl]-N'-methyl-
343632-20-2P , Acetamide, N-[2-[(2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]ethyl]-
343632-21-3P , Urea,
N-[2-[[2-(3-chlorophenyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]amino]ethyl]-N'-methyl-

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343632-69-9P , 1*H*-Pyrrolo[2,3-*d*]pyrimidin-4-amine, 2-phenyl-*N*-[2-(1*H*-pyrrol-2-yl)ethyl]-
343632-70-2P , Urea,
N-[(2*S*)-2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]cyclohexyl]-*N'*-methyl-
343632-71-3P , Urea,
N-[(1*R*)-2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]cyclohexyl]-*N'*-methyl-
343632-72-4P , Urea,
N-[(1*R*,2*S*)-2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]cyclohexyl]-*N'*-methyl-
343632-73-5P , Urea,
N-[(1*S*,2*S*)-2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]cyclohexyl]-*N'*-methyl-
343632-77-9P , Cyclopentanol, 3-[(2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, (1*S*,3*R*)-
343632-78-0P , Cyclopentanol, 3-[(2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-,
(1*R*,3*S*)- ***343632-79-1P*** , Cyclopentanol,
3-[(2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, (3*S*)- ***343633-16-9P*** ,
Cyclopentanol, 3-[(2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, (1*S*,3*S*)-
343969-79-9P , 1,2-Cyclohexanediol,
4-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, (1*R*,2*S*,4*S*)-*rel*
343969-97-1P , 1,2-Cyclopentanediol,
4-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]-, (1 α ,2 α ,4 β)

RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. and use of substituted 7*H*-pyrrolo[2,3-*b*]pyrimidines as selective adenosine A₁, A_{2a} and A₃ receptor antagonists)

IT ***343632-96-2P*** , Carbamic acid,
[2-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]ethyl]-, 1,1-dimethylethyl ester
343632-97-3P , Glycine, *N*-[(1,1-dimethylethoxy)carbonyl]-,
(1*R*,3*S*)-3-[(5,6-dimethyl-2-phenyl-1*H*-pyrrolo[2,3-*d*]pyrimidin-4-yl)amino]cyclopentyl ester, *rel*-
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and use of substituted 7*H*-pyrrolo[2,3-*b*]pyrimidines as selective adenosine A₁, A_{2a} and A₃ receptor antagonists)

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L3 ANSWER 11 OF 30 HCAPLUS COPYRIGHT 2004 ACS

ED Entered STN: 08 Jun 2001

ACCESSION NUMBER: 2001:416773 HCAPLUS

DOCUMENT NUMBER: 135:46190

TITLE: Synthesis and use of substituted pyrrolo[2,3-b]pyrimidines as selective adenosine A₁, A_{2a} and A₃ receptor antagonists

INVENTOR(S): Castelhana, Arlindo L.; McKibben, Bryan; Witter, David J.

PATENT ASSIGNEE(S): Osi Pharmaceuticals, Inc., USA

SOURCE: PCT Int. Appl., 368 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

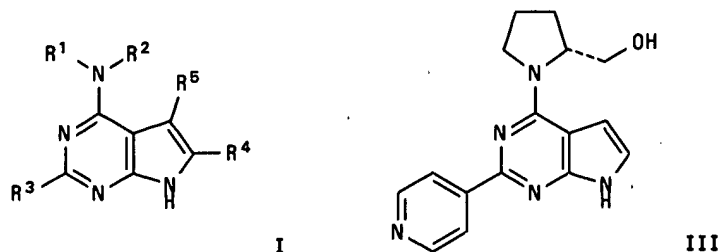
FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WD 2001039777	A1	20010607	WD 2000-US32702	20001201
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6686366	B1	20040203	US 1999-454075	19991202
EP 1246623	A1	20021009	EP 2000-988011	20001201
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003519102	T2	20030617	JP 2001-541509	20001201
PRIORITY APPLN. INFO.:				
			US 1999-454074 A	19991202
			US 1999-454075 A	19991202
			US 1999-454254 A	19991202
			US 1998-87702P P	19980602
			US 1999-123216P P	19990308
			US 1999-126527P P	19990326
			WO 1999-US12135 A2	19990601
			WO 2000-US32702 W	20001201

OTHER SOURCE(S): MARPAT 135:46190

L3 ANSWER 11 OF 30 HCAPLUS COPYRIGHT 2004 ACS
GI



AB The synthesis of compds. I, their binding to adenosine receptors and use are described [wherein; R¹, R² = H, (un)substituted alkyl or NR¹R² = (un)substituted 4-8 membered ring; R³ = (un)substituted 4-6 membered (arom.) ring; R⁴, R⁵ = H, (un)substituted alkyl, aryl (with some exceptions)]. Over 100 examples are provided. Intermediate 4-chloro-7H-pyrrolo[2,3-d]pyrimidines were prepd. by several routes from appropriately substituted cyano-pyrroles. Thus, 4-chloro-2-(4-pyridyl)-7H-pyrrolo[2,3-d]pyrimidine hydrochloride was reacted with D-prolinol (2.3 mol equiv) in DMSO at 120°C for 18 h to yield III in 13% yield after purifn. Compd. I [R¹ = AcNHCH₂CH₂; R² = H; R³ = Ph; R⁴, R⁵ = Me; II] exhibited selective binding to adenosine receptor A₁ with IC₅₀ = 82.8 nM. Compd. II also had K_i = 9.8 nM (vs. K_i = 7.1 for control ligand 8-cyclopentyl-1,3-dipropylxanthine (DPCPX)). Pyrimidine III binds 5 times more selectively to adenosine receptor A_{2a} than A₁, A_{2b} or A₃ (no data). Compd. I [R¹ = AcNH(CH₂)₄; R² = H; R³ = Ph; R⁴, R⁵ = Me] is 10 times more selective for A₃ than the other receptor subtypes. ClogP (calcd. partition coeff. between octanol and H₂O) values were detd. for selected example compds. Claimed uses of I includes administration of a systemic formulation (i.e. ophthalmic) for the treatment of a disease assocd. with A₁, A_{2a}, and A₃ adenosine receptors in a subject.

IT ***251946-19-7P***

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BYP (Byproduct); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(prepn. and use of substituted 7H-pyrrolo[2,3-b]pyrimidines as selective adenosine A₁, A_{2a} and A₃ receptor antagonists)

IT ***251946-18-6P***

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(prepn. and use of substituted 7H-pyrrolo[2,3-b]pyrimidines as selective adenosine A₁, A_{2a} and A₃ receptor antagonists)

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IT	***246855-41-4P***	***246855-42-5P***	***251945-90-1P***
	251945-91-2P	***251945-92-3P***	***251945-93-4P***
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	251946-04-0P	***251946-05-1P***	***251946-06-2P***
	251946-07-3P	***251946-08-4P***	***251946-09-5P***
	251946-10-8P	***251946-11-9P***	***251946-12-0P***
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	251946-16-4P	***251946-17-5P***	***251946-20-0P***
	251946-21-1P	***251946-22-2P***	***251946-23-3P***
	251946-24-4P	***251946-25-5P***	***251946-26-6P***
	251946-27-7P	***251946-28-8P***	***251946-29-9P***
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	251946-42-6P	***251946-43-7P***	***251946-44-8P***
	251946-45-9P	***251946-46-0P***	***251946-47-1P***
	251946-48-2P	***251946-49-3P***	***251946-50-6P***
	251946-52-8P	***251946-54-0P***	***251946-55-1P***
	251946-56-2P	***251946-57-3P***	***251946-58-4P***
	251946-59-5P	***251947-22-5P***	***251947-24-7P***
	343631-95-8P	***343631-96-9P***	***343631-97-0P***
	343631-99-2P	***343632-03-1P***	***343632-04-2P***
	343632-05-3P	***343632-06-4P***	***343632-07-5P***
	343632-08-6P	***343632-09-7P***	***343632-10-0P***
	343632-11-1P	***343632-12-2P***	***343632-13-3P***
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	343632-17-7P	***343632-19-9P***	***343632-20-2P***
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	343632-69-9P	***343632-70-2P***	***343632-71-3P***
	343632-72-4P	***343632-73-5P***	***343632-77-9P***
	343632-78-0P	***343632-79-1P***	***343633-16-9P***
	343969-79-9P	***343969-97-1P***	

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

L3 ANSWER 11 OF 30 HCAPLUS COPYRIGHT 2004 ACS

(prepn. and use of substituted 7H-pyrrolo[2,3-b]pyrimidines as selective adenosine A₁, A_{2a} and A₃ receptor antagonists)

IT ***343632-96-2P*** ***343632-97-3P***

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and use of substituted 7H-pyrrolo[2,3-b]pyrimidines as selective adenosine A₁, A_{2a} and A₃ receptor antagonists)

REFERENCE COUNT:

1

THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 12 OF 30 HCAPLUS COPYRIGHT 2004 ACS

ED Entered STN: 14 Nov 2000

ACCESSION NUMBER: 2000:792835 HCAPLUS

DOCUMENT NUMBER: 134:100695

TITLE: 7-Deazaadenines Bearing Polar Substituents: Structure-Activity Relationships of New A₁ and A₃ Adenosine Receptor Antagonists

AUTHOR(S): Hess, Sonja; Mueller, Christa E.; Frobenius, Wolfram; Reith, Ulrike;

Klotz, Karl-Norbert; Eger, Kurt

CORPORATE SOURCE: Pharmaceutical Chemistry Institute of Pharmacy, University of Leipzig, Leipzig, D-04103, Germany

SOURCE: Journal of Medicinal Chemistry (2000), 43(24), 4636-4646

CODEN: JMCMAR; ISSN:0022-2623

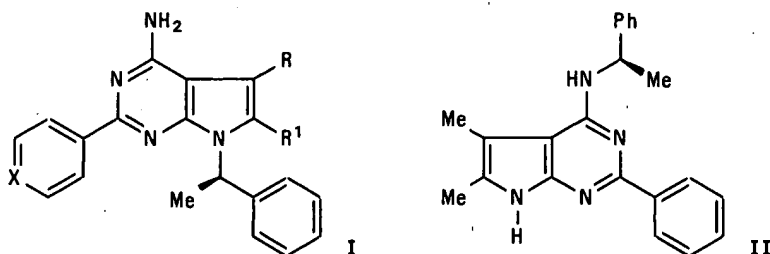
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 134:100695

GI



AB A series of 28 new pyrrolo[2,3-d]pyrimidine-4-amines, pyrimido[4,5-b]indole-4-amines, and tetrahydropyrimido[4,5-b]indole-4-amines was synthesized and their adenosine receptor affinity detd. in radioligand binding assays at rat A₁ and A_{2A} adenosine receptors (ARs). Selected compds. were addnl. investigated in binding assays at recombinant A₃ ARs. The 2-Ph residue in (R)-7-(1-methylbenzyl)-2-phenylpyrrolo[2,3-d]pyrimidine-4-amine (ADPEP) I (R = R¹ = Me, X = CH) and in the corresponding pyrimido[4,5-b]indole (APEPI) I (RR¹ = CH:CHCH:CH, X = CH) could be bioisosterically replaced by heterocyclic rings, such as 2-thienyl and 4-pyridyl. The resulting compds. retained high affinity and selectivity for A₁ ARs. Judging from the investigation of selected compds., it appears that they are also potent at human A₁ ARs and selective not only vs. A_{2A} ARs but also highly selective vs. A_{2B} and A₃ ARs. The p-pyridyl-substituted derivs. I (R = R¹ = Me, X = N) and (APPPI) I (RR¹ = CH:CHCH:CH, X = X) may be interesting pharmacol. tools due to their fluorescent properties. Pyrrolo[2,3-d]pyrimidine-4-amine derivs. which were simultaneously substituted at N7 and N4, combining the substitution pattern of ADPEP and DPEAP (II), showed very low affinity for

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A₁ ARs. This finding supports previously published hypothesis of different binding modes for pyrrolopyrimidines, such as ADPEP and DPEAP. DPEAP was found to exhibit high affinity for human A₃ ARs (K_i = 28 nM), whereas N⁴-unsubstituted analogs were inactive. DPEAP and related compds. provide new leads for the development of antagonists for the human A₃ AR.

IT ***130147-80-7*** ***177499-40-0***

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)

(prepn. of 7-deazaadenines bearing polar substituents and their structure-activity relationships as A₁ and A₃ adenosine receptor antagonists)

IT ***319481-19-1P*** ***319481-20-4P*** ***319481-21-5P***

319481-22-6P ***319481-23-7P*** ***319481-24-8P***

319481-25-9P ***319481-26-0P***

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of 7-deazaadenines bearing polar substituents and their structure-activity relationships as A₁ and A₃ adenosine receptor antagonists)

IT ***319481-39-5P*** ***319481-41-9P*** ***319481-47-5P***

319481-48-6P ***319481-49-7P*** ***319481-50-0P***

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(prepn. of 7-deazaadenines bearing polar substituents and their structure-activity relationships as A₁ and A₃ adenosine receptor antagonists)

REFERENCE COUNT: 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L3 ANSWER 13 OF 30 HCAPLUS COPYRIGHT 2004 ACS

ED Entered STN: 10 Dec 1999

ACCESSION NUMBER: 1999:783937 HCAPLUS

DOCUMENT NUMBER: 132:22973

TITLE: Preparation of pyrrolo[2,3-d]pyrimidines as adenosine receptor antagonists

INVENTOR(S): Castelhana, Arlindo L.; McKibben, Bryan; Witter, David J.

PATENT ASSIGNEE(S): Cadus Pharmaceutical Corp., USA

SOURCE: PCT Int. Appl., 169 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

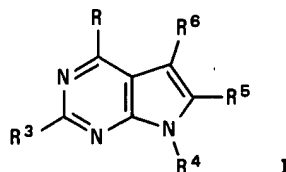
FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 9962518	A1	19991209	WO 1999-US12135	19990601
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2334200	AA	19991209	CA 1999-2334200	19990601
AU 9942265	A1	19991220	AU 1999-42265	19990601
AU 763658	B2	20030731		
BR 9911612	A	20010206	BR 1999-11612	19990601
EP 1082120	A1	20010314	EP 1999-926107	19990601
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2002516861	T2	20020611	JP 2000-551774	19990601
US 6686366	B1	20040203	US 1999-454075	19991202
NO 2000006090	A	20010131	NO 2000-6090	20001130
US 2002028782	A1	20020307	US 2000-728229	20001201
PRIORITY APPLN. INFO.:				
			US 1998-87702P P	19980602
			US 1999-123216P P	19990308
			US 1999-126527P P	19990326
			WO 1999-US12135 W	19990601

OTHER SOURCE(S): MARPAT 132:22973

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AB Title compds. [I; R = NR¹R²; R¹-R⁴ = H, alkyl, aryl, etc.; NR¹R² = heterocyclyl; R⁵,R⁶ = H, halo, alkyl, aryl, etc.; R⁴R⁵,R⁵R⁶ = atoms to complete a ring] were prepd. Thus, 2-amino-3-cyano-4,5-dimethyl-1-(1-phenylethyl)pyrrole was N-benzoylated and the product cyclized to give, after deprotection and chlorination, I (R³ = Ph, R⁴ = H, R⁵ = R⁶ = Me)(II; R = Cl) which was aminated by trans-4-hydroxycyclohexylamine to give II (R = trans-4-hydroxycyclohexylamino). Data for biol. activity of I were given.

IT	***246855-41-4P***	***246855-42-5P***	***251945-90-1P***
	251945-91-2P	***251945-92-3P***	***251945-93-4P***
	251945-94-5P	***251945-95-6P***	***251945-96-7P***
	251945-97-8P	***251945-98-9P***	***251945-99-0P***
	251946-00-6P	***251946-01-7P***	***251946-03-9P***
	251946-04-0P	***251946-05-1P***	***251946-06-2P***
	251946-07-3P	***251946-08-4P***	***251946-09-5P***
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RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified);

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SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation);
USES (Uses)

(prepn. of pyrrolo[2,3-d]pyrimidines as adenosine receptor antagonists)

IT ***251947-22-5P*** ***251947-24-7P***

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or
reagent)

(prepn. of pyrrolo[2,3-d]pyrimidines as adenosine receptor antagonists)

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 14 OF 30 HCAPLUS COPYRIGHT 2004 ACS

ED Entered STN: 13 Oct 1999

ACCESSION NUMBER: 1999:650392 HCAPLUS

DOCUMENT NUMBER: 131:271765

TITLE: Preparation of new cephalosporin derivatives as anti-bacterial agents

INVENTOR(S): Takagi, Hiroyasu; Yotsuji, Minako; Kanna, Hiroshi; Matsukura, Hiroko; Murakami, Makoto; Suzuki, Keisuke; Minami, Shinzaburo; Watanabe, Yasuo

PATENT ASSIGNEE(S): Toyama Chemical Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 53 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

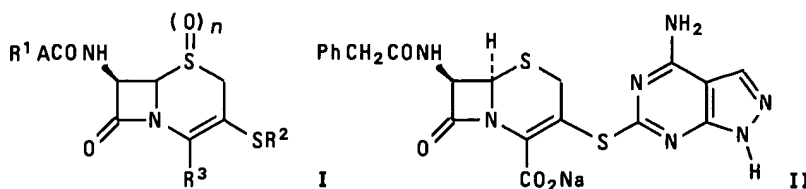
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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JP 11279180	A2	19991012	JP 1999-13670	19990122
PRIORITY APPLN. INFO.:			JP 1998-26582	19980123
			JP 1998-33597	19980130

OTHER SOURCE(S): MARPAT 131:271765

GI



AB Cephalosporin derivs. of formula I [R¹ = H, halo, CN, alkyl, alkoxy, alkylcarbonyloxy, etc.; A = CH₂, cycloalkylidene, vinylidene, etc.; R² = heteroaryl, etc.; R³ = CO₂H, carboxylate; n = 0, 1] are prep'd. as antibacterial agents. Thus, 4-aminopyrazolo[3,4-d]pyrimidin-6-ylthiol was added to 7-phenylacetamide-3-trifluorosulfonyloxy-3-cephem-4-carboxylic acid diphenylmethyl ester 1β-oxide, then transformed into II. The MIC value of II against *S. aureus* FDA 209P was 0.2 μg/mL. Pharmaceutical compns. contg. I are described.

IT ***245487-76-7P*** ***245488-78-2P*** ***245488-81-7P***

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

L3 ANSWER 14 OF 30 HCAPLUS COPYRIGHT 2004 ACS

(prepn. of cephalosporin derivs. as antibacterial agents)

IT ***245486-48-0P*** ***245487-14-3P*** ***245488-25-9P***

245488-28-2P ***245488-50-0P*** ***245488-54-4P***

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of cephalosporin derivs. as antibacterial agents)

L3 ANSWER 15 OF 30 HCAPLUS COPYRIGHT 2004 ACS

ED Entered STN: 09 Sep 1999

ACCESSION NUMBER: 1999:571295 HCAPLUS

DOCUMENT NUMBER: 131:281026

TITLE: Selective A₁-adenosine receptor antagonists identified using yeast *Saccharomyces cerevisiae* functional assays

AUTHOR(S): Campbell, Robert M.; Cartwright, Craig; Chen, Wei; Chen, Yong; Duzic, Emir; Fu, Jian-Min; Loveland, Michelle; Manning, Ron; McKibben, Bryan; Pleiman, Christopher M.; Silverman, Lauren; Trueheart, Joshua; Webb, David R.; Wilkinson, Vicki; Witter, David J.; Xie, Xiaobing; Castelano, Arlindo L.

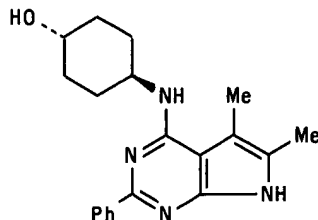
CORPORATE SOURCE: Cadus Pharmaceutical Corporation, Tarrytown, NY, 10591, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (1999), 9(16), 2413-2418
CODEN: BMCLE8; ISSN:0960-894X

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



I

AB Evaluation of a biased "library" of pyrrolo[2,3-d]pyrimidines using yeast-based functional assays expressing human A₁- and A_{2a}-adenosine receptors, led to the A₁ selective antagonist I.

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A direct correlation between yeast functional activity and binding data was established. Practical compds. with polar residues at C-4 of the pyrrolopyrimidine system required H-bond donor functionality for high potency.

IT ***177499-40-0P*** ***246855-41-4P*** ***246855-42-5P***
246855-43-6P ***246855-44-7P*** ***246855-45-8P***
246855-46-9P ***246855-47-0P*** ***246855-48-1P***

RL: BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)

(selective A₁-adenosine receptor antagonists identified using yeast functional assays)

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L3 ANSWER 16 OF 30 HCAPLUS COPYRIGHT 2004 ACS

ED Entered STN: 07 Jan 1999

ACCESSION NUMBER: 1999:9714 HCAPLUS

DOCUMENT NUMBER: 130:71627

TITLE: Compositions and methods for preventing restenosis following
revascularization procedures

INVENTOR(S): Martin, Pauline L.; McAfee, Donald A.

PATENT ASSIGNEE(S): Discovery Therapeutics, Inc., USA

SOURCE: PCT Int. Appl., 26 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WD 9857651	A1	19981223	WD 1998-US12717	19980618
W: AU, CA, JP, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9880740	A1	19990104	AU 1998-80740	19980618
AU 740770	B2	20011115		
EP 1014995	A1	20000705	EP 1998-929099	19980618
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
JP 2002505687	T2	20020219	JP 1999-504810	19980618
US 6372723	B1	20020416	US 1999-456432	19991208
US 2001009907	A1	20010726	US 2001-783032	20010215
US 6339072	B2	20020115		

PRIORITY APPLN. INFO.:

US 1997-50031P P 19970618

WD 1998-US12717 W 19980618

US 1999-456432 A3 19991208

AB In the present invention, a method is provided which reduces or prevents restenosis following revascularization procedures. It has now been found that selective stimulation of adenosine A_{2A} receptors can reduce or prevent such restenosis. This method may be achieved either by: (a) the administration of selective adenosine A_{2A} receptor agonists, (b) the administration of a selective adenosine A₁ antagonist in combination with either a selective adenosine A_{2A} receptor agonist or a non-selective adenosine agonist, or (c) the administration of a selective adenosine A₁ antagonist in order to block adenosine A₁ receptor activation by endogenously-released adenosine. The present invention is also directed to an improved surgical procedure that relies upon selective stimulation of adenosine A_{2A} receptors. The degree of arterial stenosis in rabbits after angioplasty treated with the adenosine A_{2A} selective agonist 2-cyclohexylmethylenhydrazinoadenosine was significantly less than arterial

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stenosis in rabbits treated with vehicle.

IT ***130147-80-7***

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(comps. for preventing restenosis following revascularization procedures)

REFERENCE COUNT:

2

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 17 OF 30 HCAPLUS COPYRIGHT 2004 ACS

ED Entered STN: 27 Apr 1998

ACCESSION NUMBER: 1998:239113 HCAPLUS

DOCUMENT NUMBER: 128:299556

TITLE: Compositions and methods for modulating melanin production

INVENTOR(S): Manneth, Victor; Patel, Rajesh

PATENT ASSIGNEE(S): Therasys, Inc., USA; Manneth, Victor; Patel, Rajesh

SOURCE: PCT Int. Appl., 26 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9815276	A1	19980416	WO 1997-US18148	19971008
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
US 5998423	A	19991207	US 1997-940338	19970930
CA 2242525	AA	19980416	CA 1997-2242525	19971008
AU 9746728	A1	19980505	AU 1997-46728	19971008
EP 880353	A1	19981202	EP 1997-945558	19971008
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
NZ 330862	A	20000728	NZ 1997-330862	19971008
JP 2002515885	T2	20020528	JP 1998-517708	19971008

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L3 ANSWER 17 OF 30 HCAPLUS COPYRIGHT 2004 ACS

PRIORITY APPLN. INFO.:

US 1996-27944P P 19961008

US 1997-940338 A 19970930

WO 1997-US18148 W 19971008

OTHER SOURCE(S): MARPAT 128:299556

AB Compns. and methods for the modulation of melanin prodn. are provided in which the active component is an adenosine receptor antagonist or agonist. A formulation for topical delivery of 8-cyclopentyl-1,3-dimethylxanthine was prepd.

IT ***206197-05-9***

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(compns. for modulating melanin prodn.)

REFERENCE COUNT:

2

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 18 OF 30 HCAPLUS COPYRIGHT 2004 ACS

ED Entered STN: 31 Jul 1997

ACCESSION NUMBER: 1997:478038 HCAPLUS

DOCUMENT NUMBER: 127:156859

TITLE: Interest of cluster significance analysis in structure-affinity relationships for non-xanthine heterocyclic antagonists of adenosine

AUTHOR(S): Adenot, M.; Benezech, V.; Bompert, J.; Bonnet, P. A.; Chapat, J. P.; Grassy, G.

CORPORATE SOURCE: Centre de Biochimie Structurale, UMR CNRS 9955, INSERM U414, Faculte de Pharmacie, Montpellier, 34060, Fr.

SOURCE: European Journal of Medicinal Chemistry (1997), 32(6), 493-504
CODEN: EJMCA5; ISSN:0223-5234

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

AB To define some predictive rules for the discrimination of adenosine antagonists by their A₁-receptor affinity, the authors performed a systematic QSAR anal. As no significant descriptors of affinity were found, the authors then proposed to introduce a calcd. enthalpy or entropy change for the interaction as a first approxn. of the affinity descriptors. Since the structural details of the common receptor binding site remain to be detd., an indirect strategy was utilized involving the simulation of amino acid residues that are thought to interact with the ligand. Estg. enthalpic and entropic components by means of a semi-empirical quantum mech. AM1 force calcn., the authors found a significant clustering of enthalpy change values. This method provides a good descriptor of interaction and also a simple tool for testing hypotheses on the nature of putative binding sites.

IT ***130147-79-4*** ***130147-80-7***

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified);
BIOL (Biological study)

(cluster significance anal. in structure-affinity relationships for non-xanthine heterocyclic antagonists of adenosine)

L3 ANSWER 19 OF 30 HCAPLUS COPYRIGHT 2004 ACS

ED Entered STN: 12 Sep 1996

ACCESSION NUMBER: 1996:544121 HCAPLUS

DOCUMENT NUMBER: 125:237579

TITLE: New Purines and Purine Analogs as Modulators of Multidrug Resistance

AUTHOR(S): Dhainaut, Alain; Regnier, Gilbert; Tizot, Andre; Pierre, Alain; Leonce, Stephane; Guilbaud, Nicolas; Kraus-Berthier, Laurence; Atassi, Ghanem

CORPORATE SOURCE: Institut de Recherches Servier, Suresnes, 92150, Fr.

SOURCE: Journal of Medicinal Chemistry (1996), 39(20), 4099-4108

CODEN: JMCMAR; ISSN:0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A series of 36 purine and purine analog derivs. have been synthesized and tested for their ability to modulate multidrug resistance in vitro (P388/VCR-20 and KB-A1 cells) and in vivo (P388/VCR leukemia). Compds. were compared to S9788, a triazine deriv. which has already shown some activity during phase 1 clin. trials and also a limiting cardiovascular side effect possibly linked to its calcium channel affinity. The fact that active compds. increase adriamycin accumulation in the resistant KB-A1 cells, and not in the sensitive KB-3-1 cells, suggests they act predominantly by inhibiting the P-glycoprotein-catalyzed efflux of cytotoxic agents. No direct relation was found between the affinity for the phenylalkylamine binding site of the calcium channel and in vitro sensitization of resistant cells. In vivo, when administered po in assocn. with vincristine (0.25 mg/kg), five of the compds., of very differing calcium channel affinities (K_i from 5 to 560 nM), fully restored ($T/V \geq 1.4$) the sensitivity of P388/VCR leukemia to vincristine.

IT ***181862-15-7P*** ***181862-16-8P***

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; prepn. of new purines and purine analogs as modulators of multidrug resistance)

IT ***157838-12-5P***

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of new purines and purine analogs as modulators of multidrug resistance)

L3 ANSWER 20 OF 30 HCAPLUS COPYRIGHT 2004 ACS

ED Entered STN: 23 Jul 1996

ACCESSION NUMBER: 1996:432308 HCAPLUS

DOCUMENT NUMBER: 125:157747

TITLE: Theoretical structure-activity studies of adenosine A₁ ligands: requirements for receptor affinity

AUTHOR(S): Dooley, Michael J.; Kono, Motomichi; Suzuki, Fumio

CORPORATE SOURCE: Pharmaceutical Res. Lab., Kyowa Hakko Kogyo Co. Ltd., Shizuoka-ken, 411, Japan

SOURCE: Bioorganic & Medicinal Chemistry (1996), 4(6), 923-934

CODEN: BMECEP; ISSN:0968-0896

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The three-dimensional (3-D) requirements for A₁ adenosine receptor affinity have been studied based on hydrogen-bonding functionality correlation between a group of twelve A₁ adenosine receptor ligands representing ten structurally different classes of compds. Electrostatic potential similarity indexes and shape similarity indexes strongly support the proposed receptor-bound orientations of the ligands. We conclude, in areas common to both agonist and antagonist binding at the A₁ receptor, that the ligands are recognized by a similar physicochem. 3-D environment. The finding of similar 3-D requirements for agonists and antagonists suggests a fairly static receptor structure in the region common to agonist and antagonist binding. The ribose moiety is remote from antagonist binding site. Such a 3-D environment rationalizes the binding of a no. of potent novel antagonists including KW-3902, not previously reported in modeling studies.

IT ***130147-80-7***

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)

(theor. structure-activity studies of adenosine A₁ ligands: requirements for receptor affinity)

L3 ANSWER 21 OF 30 HCAPLUS COPYRIGHT 2004 ACS

ED Entered STN: 23 Jul 1996

ACCESSION NUMBER: 1996:432307 HCAPLUS

DOCUMENT NUMBER: 125:157746

TITLE: Conformational search for the N⁶-substituted adenosine analogs and related adenosine A₁ receptor antagonists

AUTHOR(S): Dooley, Michael L.; Kono, Motomichi; Suzuki, Fumio

CORPORATE SOURCE: Pharmaceutical Res. Lab., Kyowa Hakko Kogyo Co. Ltd., Shizuoka-ken, 411, Japan

SOURCE: Bioorganic & Medicinal Chemistry (1996), 4(6), 917-921

CODEN: BMECEP; ISSN:0968-0896

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The search for 3-D requirements for the adenosine A₁ receptor affinity is useful to aid in the design of more potent and/or novel ligands as pharmacol. tools and therapeutics for the receptor. To emboss 3-D requirements for adenosine A₁ receptor affinity among adenosine receptor antagonists, adenosine and xanthine analogs, conformations for the N⁶-substituted adenosine analogs and related adenosine A₁ receptor antagonists were thoroughly searched by semi-empirical quantum mechanics calcns. Newly established global min. for these compds. (C1'-N⁶-C6-N1 torsion: 10°) are consistent with retrieved structures from Cambridge Structural Database and previously published NMR data on the soln. conformation of N⁶-substituted adenosine analogs. However, these newly studied global min. for adenosine analogs are different from those previously reported (C1'-N⁶-C6-N1 torsion: ±75°).

IT ***130147-80-7***

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)

(conformational search for the N⁶-substituted adenosine analogs and related adenosine A₁ receptor antagonists)

L3 ANSWER 22 OF 30 HCAPLUS COPYRIGHT 2004 ACS

ED Entered STN: 06 Jun 1996

ACCESSION NUMBER: 1996:328283 HCAPLUS

DOCUMENT NUMBER: 125:25634

TITLE: Chiral Pyrrolo[2,3-d]pyrimidine and Pyrimido[4,5-b]indole Derivatives:
Structure-Activity Relationships of Potent, Highly Stereoselective
A₁-Adenosine Receptor Antagonists

AUTHOR(S): Mueller, Christa E.; Geis, Uli; Grahner, Bettina; Lanzner, Wolfgang;
Eger, Kurt

CORPORATE SOURCE: Institut fuer Pharmazie und Lebensmittelchemie Pharmazeutische
Chemie, Julius-Maximilians-Universitaet, Wuerzburg, D-97074, Germany

SOURCE: Journal of Medicinal Chemistry (1996), 39(13), 2482-2491

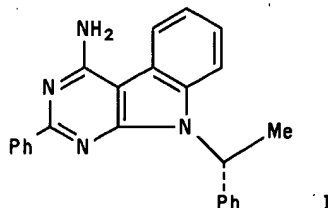
CODEN: JMCMAR; ISSN:0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

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AB A series of novel, mostly chiral pyrrolo[2,3-d]pyrimidine and pyrimido[4,5-b]indole derivs. has been synthesized and investigated in radioligand binding assays at the high-affinity adenosine receptor (AR) subtypes A₁ and A_{2a}. The compds. can be envisaged as adenine and hypoxanthine analogs lacking the nitrogen in the 7-position (7-deazaadenines and 7-deazahypoxanthines). 7-Deazaadenines were much more potent than 7-deazahypoxanthines at AR with A₁AR affinities in the low-nanomolar range, extraordinarily high selectivity for the rat brain A₁AR vs. the A_{2a}AR (several thousand-fold), and high stereoselectivity (up to 96-fold). Pyrimido[4,5-b]indoles were more potent A₁AR antagonists compared to pyrrolo[2,3-d]pyrimidines. Compd. I is one of the most potent and most selective nonxanthine A₁AR antagonists known to date (K_i = 2.8 nM, >2000-fold A₁-selective). A new class of very potent A₁AR antagonists has been identified, namely, 2-phenyl-7-deazaadenines bearing a substituent at the exocyclic amino group (N⁴-substituted 2-phenyl-7-deazaadenines).

(R)-N-(1-Phenylethyl)-4-amino-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-d]pyrimidine (DPEAP) showed a K_i value of 6.7 nM at A₁AR and >4000-fold A₁ selectivity. Different binding modes are

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postulated for the N⁴-substituted 4-aminopyrrolo[2,3-d]pyrimidines and the 7-substituted derivs., based on a comparison of steric, electronic, and hydrophobic properties of the two classes of compds. Water soly. and lipophilicity have been detd. for selected compds.

4-Amino-5,6-dimethyl-2-(3-chlorophenyl)-7H-pyrrolo[2,3-d]pyrimidine showed the highest water soly./A₁AR affinity ratio of 368 in the present series, over 2000-fold A₁ selectivity, and 64-fold stereoselectivity (R > S).

IT	***130147-80-7P***	***130147-81-8P***	***177499-32-0P***
	177499-33-1P	***177499-34-2P***	***177499-35-3P***
	177499-36-4P	***177499-37-5P***	***177499-40-0P***
	177499-41-1P	***177570-32-0P***	***177570-33-1P***
	177570-34-2P	***177570-35-3P***	

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified);
SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and structure-activity of pyrroloindoles and pyrrolopyrimidines as A₁-adenosine
receptor antagonists)

L3 ANSWER 23 OF 30 HCAPLUS COPYRIGHT 2004 ACS

ED Entered STN: 21 Feb 1996

ACCESSION NUMBER: 1996:109105 HCAPLUS

DOCUMENT NUMBER: 124:249637

TITLE: A survey of nonxanthine derivatives as adenosine receptor ligands
AUTHOR(S): Siddiqi, Suhaib M.; Ji, Xiao-duo; Melman, Neli; Olah, Mark E.; Jain, Rahul; Evans, Patricia; Glashofer, Marc; Padgett, William L.; Cohen, Louis A.; et al.

CORPORATE SOURCE: Molecular Recognition Section, National Institutes of Health, Bethesda, MD, 20892, USA

SOURCE: Nucleosides & Nucleotides (1996), 15(1-3), 693-717
CODEN: NUNUD5; ISSN:0732-8311

PUBLISHER: Dekker

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The binding affinities at rat A₁, A_{2a}, and A₃ adenosine receptors of a wide range of heterocyclic derivs. have been detd. Mono-, bi-, tricyclic and macrocyclic compds. were screened in binding assays, using either [³H]PIA or [³H]CGS 21680 in rat brain membranes or [¹²⁵I]AB-MECA in CHO cells stably transfected with rat A₃ receptors. Several new classes of adenosine antagonists (e.g. 5-oxoimidazopyrimidines and a pyrazoloquinazoline) were identified. Various sulfonylpiperazines, 11-hydroxytetrahydrocarbazolenine, 4H-pyrido[1,2-a]pyrimidinone, folic acid, and cytochalasin H and J bound to A₃ receptors selectively. Moreover, cytochalasin A, which bound to A₁ adenosine receptors with K_i value of 1.9 μM, inhibited adenylyl cyclase in rat adipocytes, but not via reversible A₁ receptor binding.

IT ***111601-39-9***

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(nonxanthine derivs. as adenosine receptor ligands)

L3 ANSWER 24 OF 30 HCAPLUS COPYRIGHT 2004 ACS

ED Entered STN: 05 Oct 1995

ACCESSION NUMBER: 1995:833632 HCAPLUS

DOCUMENT NUMBER: 123:313913

TITLE: A One-Step Ring Transformation/Ring Annulation Approach to Pyrrolo[2,3-d]pyrimidines. A New Synthesis of the Potent Dihydrofolate Reductase Inhibitor TNP-351

AUTHOR(S): Taylor, Edward C.; Patel, Hemantkumar H.; Jun, Jong-Gab

CORPORATE SOURCE: Department of Chemistry, Princeton University, Princeton, NJ, 08544, USA

SOURCE: Journal of Organic Chemistry (1995), 60(21), 6684-7
CODEN: JOCEAH; ISSN:0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 123:313913

AB Condensation of amidines with 2-amino-3-cyanofurans gives 2-substituted-4-aminopyrrolo[2,3-d]pyrimidines by a ring-opening, ring-recyclization sequence of reactions through which the starting furan 2-amino nitrogen becomes the pyrrole nitrogen of the final product and one of the amidine nitrogens becomes N-1 of the fused pyrimidine ring. 2,4-Diamino-5-[2-(4-carbethoxyphenyl)ethyl]pyrrolo[2,3-d]pyrimidine, a key intermediate in the synthesis of the dihydrofolate reductase inhibitor TNP-351, has been prep'd. in one step by reaction of 4-[2-(2-amino-3-cyano-4-furanyl)ethyl]benzoic acid Et ester with guanidine.

IT ***170170-17-9P***

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of pyrrolo[2,3-d]pyrimidines from guanidines and (amino)furan carbonitriles)

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L3 ANSWER 25 OF 30 HCAPLUS COPYRIGHT 2004 ACS

ED Entered STN: 29 Oct 1994

ACCESSION NUMBER: 1994:605381 HCAPLUS

DOCUMENT NUMBER: 121:205381

TITLE: Preparation of purine derivatives and analogs as agents for suppressing tumor cell resistance to antineoplastic agents

INVENTOR(S): Regnier, Gilbert; Dhainaut, Alain; Atassi, Ghanem; Pierre, Alain

PATENT ASSIGNEE(S): Adir et Compagnie, Fr.

SOURCE: PCT Int. Appl., 30 pp

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

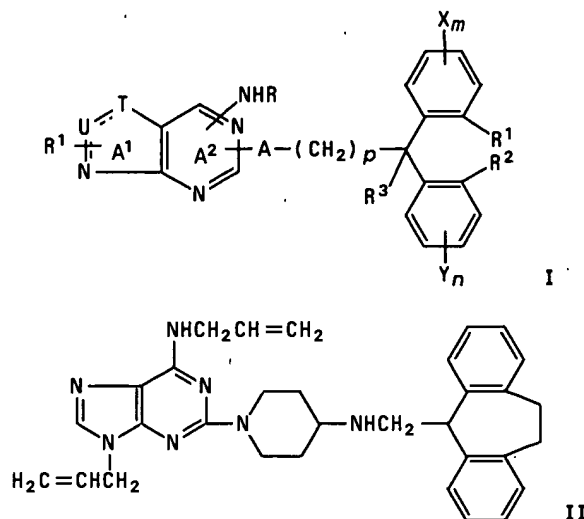
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	----	-----	-----	-----
WO 9413668	A1	19940623	WO 1993-FR1211	19931209
W: AU, CA, JP, NZ, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
FR 2699176	A1	19940617	FR 1992-14913	19921211
FR 2699176	B1	19950303		
CA 2117462	AA	19940623	CA 1993-2117462	19931209
AU 9456535	A1	19940704	AU 1994-56535	19931209
AU 666422	B2	19960208		
EP 673376	A1	19950927	EP 1994-902003	19931209
EP 673376	B1	19960522		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
JP 08504426	T2	19960514	JP 1993-513866	19931209
AT 138380	E	19960615	AT 1994-902003	19931209
ES 2091126	T3	19961016	ES 1994-902003	19931209
US 5508277	A	19960416	US 1994-284689	19940810
PRIORITY APPLN. INFO.:				
			FR 1992-14913	19921211
			WO 1993-FR1211	19931209

OTHER SOURCE(S): MARPAT 121:205381

GI

L3 ANSWER 25 OF 30 HCAPLUS COPYRIGHT 2004 ACS



AB The title compds. I [T and U represent CH or N, and rings A¹ and A² together form purine ring, pyrazolo[3,4-d]pyrimidine, etc.; R, R' = alkyl, alkenyl; A = heteromonocyclic moiety (further details on said heteromonocyclic moiety are given); p = 0 or 1; X, Y = H, halo, etc.; m, n = 1 - 3; R¹, R² = H, alkyl; or R¹R² = O, (CH₂)_x, etc; x = 1 - 3; R³ = H, Ph] are prepd. Purine deriv. II was prepd. from 2,6-dichloropurine in multiple steps. Mice with transplanted tumor were dosed with II (25 mg/Kg i.p.) and vincristine (0.50 mg/kg i.p.). The survival time of said mice was 1.54 times survival time of mice with tumor receiving vincristine therapy.

IT ***157838-12-5P***

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of, as agent for suppressing tumor cell resistance to antineoplastic agents)

L3 ANSWER 26 OF 30 HCAPLUS COPYRIGHT 2004 ACS

ED Entered STN: 08 Dec 1990

ACCESSION NUMBER: 1990:611696 HCAPLUS

DOCUMENT NUMBER: 113:211696

TITLE: 7-Deaza-2-phenyladenines: structure-activity relationships of potent A₁ selective adenosine receptor antagonists

AUTHOR(S): Mueller, Christa E.; Hide, Izumi; Daly, John W.; Rothenhaeusler, Klaus; Eger, Kurt

CORPORATE SOURCE: Lab. Bioorg. Chem., Natl. Inst. Diabetes, Dig. Kidney Dis., Bethesda, MD, 20892, USA

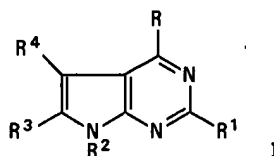
SOURCE: Journal of Medicinal Chemistry (1990), 33(10), 2822-8
CODEN: JMCMAR; ISSN:0022-2623

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 113:211696

GI



AB 7-Deazapurines I [R = NH₂, Cl, OH, SH, SMe, SO₂Me; R¹ = H, SH, SMe, SO₂Me, Me, Ph, 4-ClC₆H₄; R² = H, Ph, hexyl, allyl, 2,3-(MeO)₂C₆H₃, 4-BrC₆H₄CH₂, 2-deoxyribosyl, CHMePh; R³ = R⁴ = Me, H, CHO, CO₂H; R³R⁴ = (CH₂)₄, CH:CHCH:CH] were prep'd. in an attempt to improve the adenosine receptor affinity and A₁ or A₂ selectivity. The adenosine receptor affinities were assessed by measuring the inhibition of [³H]-(R)-N-(phenylisopropyl)adenosine (II) binding to rat brain A₁ and inhibition of [³H]-5'-(N-ethylcarboxamido)adenosine (III) binding to rat striatum A₂ adenosine receptors. Selected I were further exam'd. in adenosine receptor coupled adenylate cyclase assays. All tested comp'ds. antagonized the inhibition of adenylate cyclase elicited by interaction of II with A₁ receptors in rat fat cell membranes and the activation of adenylate cyclase elicited by interaction of III with A₂ receptors of pheochromocytoma PC12 cell membranes. The results indicate that 7-deazahypoxanthines have a potential for A₂ selectivity, while all 7-deazaadenines are A₁ selective. Introduction of a Ph residue in the 2-position of 7-deazaadenines increases A₁ activity tremendously. Thus, I (R = NH₂, R = 4-ClC₆H₄, R² = Ph, R³ = R⁴ = Me) is potent and specific for the A₁ receptors of rat brain (K_i = 122 nM), having no affinity for the A₂ receptors of rat striatum. The comp'd. has low activity at the A₂ receptors of rat PC12 cell membranes where it appears to act as a noncompetitive inhibitor. The most potent A₁ antagonist was I [R = NH₂, R¹ = Ph, R² = (R)-CHMePh, R³ = R⁴ = Me].

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IT ***111601-39-9*** ***111601-40-2*** ***130147-78-3***
 130147-79-4 ***130147-80-7*** ***130147-81-8***
 130147-82-9 ***130147-83-0***

RL: RCT (Reactant); RACT (Reactant or reagent)
 (adenosine receptor antagonist activity of)

L3 ANSWER 27 OF 30 HCAPLUS COPYRIGHT 2004 ACS

ED Entered STN: 28 Oct 1988

ACCESSION NUMBER: 1988:549471 HCAPLUS

DOCUMENT NUMBER: 109:149471

TITLE: Phosphorus pentoxide in organic synthesis. XXXVI. Synthesis of
 7H-pyrrolo[2,3-d]pyrimidine-2,4-diamines and 7-diazaisoguanines from
 7H-pyrrolo[2,3-d]pyrimidine-2,4-diones

AUTHOR(S): Joergensen, Anker; Moharram, H. H.; Pedersen, Erik B.

CORPORATE SOURCE: Dep. Chem., Odense Univ., Odense, DK-5230, Den.

SOURCE: Chemica Scripta (1988), 28(2), 201-4

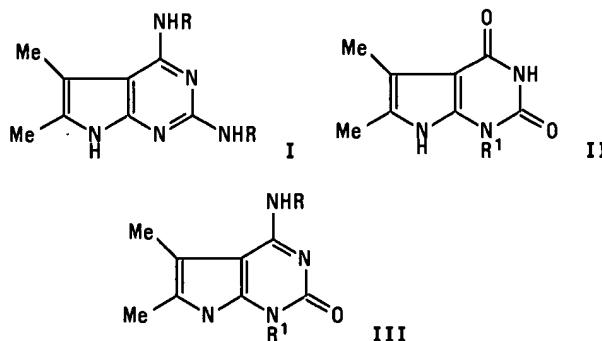
CODEN: CSRPB9; ISSN:0004-2056

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 109:149471

GI



AB Diaryldimethylpyrrolopyrimidinediamines I (R = Ph, *m*-tolyl, *p*-tolyl, C₆H₄Bu-*p*, 3,5-xylyl) were prepd. in ca. 20% yield by heating dimethylpyrrolopyrimidinedione II (R¹ = H) with a mixt. of P₂O₅, Et₃N.HCl, and RNH₂ in a 1:4:4 molar ratio. Under similar reaction conditions II (R¹ = Me) afforded 40-50% (arylamino)pyrrolopyrimidinones III (R¹ = Me). The reaction of 1 equiv II (R¹ = H) with 8 equiv P₂O₅, Et₃N.HCl, and RNH₂ gave 35-54% III (R¹ = H).

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IT ***116673-05-3P*** ***116673-06-4P*** ***116673-07-5P***

116673-08-6P ***116673-09-7P***

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

L3 ANSWER 28 OF 30 HCAPLUS COPYRIGHT 2004 ACS

ED Entered STN: 25 Dec 1987

ACCESSION NUMBER: 1987:636656 HCAPLUS

DOCUMENT NUMBER: 107:236656

TITLE: Selected reactions on the o-aminonitrile system of substituted pyrroles

AUTHOR(S): Eger, Kurt; Pfahl, Johannes Georg; Folkers, Gerd; Roth, Hermann J.

CORPORATE SOURCE: Pharm. Inst., Univ. Tuebingen, Tuebingen, D-7400, Fed. Rep. Ger.

SOURCE: Journal of Heterocyclic Chemistry (1987), 24(2), 425-30

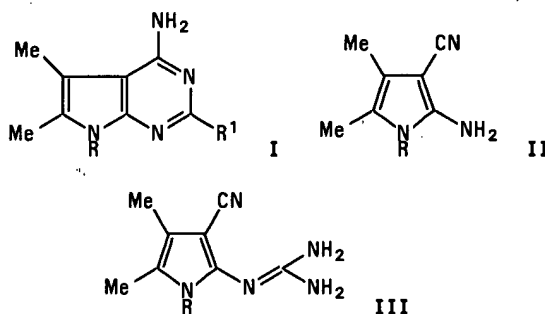
CODEN: JHTCAD; ISSN:0022-152X

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 107:236656

GI



AB Pyrrolo[2,3-*d*]pyrimidine-2,4-diamines I (R = Ph, PhCHMe, R¹ = NH₂) were prepd. from pyrroles II via amidines III. I (R = Ph, PhCHMe, R¹ = Me, Ph, *p*-ClC₆H₄) were prepd. from II and R¹CN. Some unexpected reactions on the 2-aminopyrrole-3-carbonitrile system are described.

IT ***111601-36-6P*** ***111601-37-7P***

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and deprotection of, with polyphosphoric acid)

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IT ***111601-39-9P*** ***111601-40-2P***

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

L3 ANSWER 29 OF 30 HCAPLUS COPYRIGHT 2004 ACS

ED Entered STN: 22 Apr 2001

ACCESSION NUMBER: 1962:476026 HCAPLUS

DOCUMENT NUMBER: 57:76026

ORIGINAL REFERENCE NO.: 57:15129f-i,15130a-i

TITLE: Pyrrolopyrimidine vasodilators

INVENTOR(S): Hitchings, George H.; Ledig, Kurt W.; West, Robert A.

PATENT ASSIGNEE(S): Burroughs Wellcome & Co. (U.S.A.) Inc.

SOURCE: 5 pp.

DOCUMENT TYPE: Patent

LANGUAGE: Unavailable

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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US 3037980		19620605	US	
PRIORITY APPLN. INFO.:			GB	19550818

GI For diagram(s), see printed CA Issue.

AB Pyrrolo[2,3-d]pyrimidines, having the structure I, were prepd. usually by reaction of the 4-chloro deriv. with the proper amine. 4-Chloropyrrolo [2,3-d]pyrimidine (II) (1.3 g.), 30 cc. EtOH, 1 drop concd. HCl, and 2.5 cc. PrNH₂ was heated 7 hrs. at 125°, cooled, evapd., and the residue triturated with 5 cc. 2.5% NaOH and filtered to give 1.2 g. I (R¹, R², R³ = H, R⁴ = Pr), m. 162° (30% aq. EtOH). The following I were prepd. similarly using the proper starting materials (R¹, R², R³, R⁴, and m.p. given): H, Me, H, pentyl, 167-9° (25% EtOH); Me, H, H, pentyl, 125-7° (C₆H₆-hexane); H, H, H, Me, 236°; H, H, Me, Me, 222°; H, H, Et, H, 205°; H, H, Et, Me, 170°; H, H, H, pentyl, 129°; H, H, H, CHMe₂, 169-70°; H, H, Me, Pr, 148-9°; H, H, H, CH₂CH₂OH, 209°; H, H, H, CH₂CH(OEt)₂, 124-6°; H, H, H, Bu, 145-6°; H, H, H, CH₂CHMe₂, 173-4°; H, H, H, CHMeEt, 125-6°; H, H, H, CMe₃, 183°; H, H, H, CH₂CH₂CHMe₂, 166-7°; H, H, H, CH₂CHMeEt, 140-1°; H, H, H, hexyl, 150-1°; H, H, H, heptyl, 126-7° [135° (heptane)]; H, H, H, octyl, 118-19°; H, H, H, allyl, 167°; H, H, H, CH₂CH₂NHEt, 146-7°; H, H, H, cyclopentyl, 162-3°; H, H, H, CH₂CH₂OMe, 167-8°; H, Me, H, CH₂CH₂OMe, 144-6°; H, H, H, CH₂CH₂CH₂OMe, 144-5°; H, H, Me, CHMe₂, 156-7°; H, H, Et, Et, 174-5°; H, H, Pr, Pr, 118°; H, H, H, piperidino, 184-5°; H, Me, H, Et, 189-90°; Me, H, H, Et, 159°; H, H, Me, pentyl, 133-5°. Reactions of this type with higher mol. wt. amines were carried out by refluxing in an aq. system. For example, 1.2 g. II, 5 g. nonylamine,

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and 50 cc. H₂O was refluxed 2 hrs., 4 cc. 5% NaOH added, chilled, and filtered to give 2.5 g. I (R¹, R², R³ = H, R⁴ = nonyl), hemihydrate m. 122-4° (aq. EtOH). The following compds. were prepd. similarly from the appropriate starting materials (R¹, R², R³, R⁴, m.p. given): H, Me, H, benzyl, 205-7°; H, Me, H, N-methylpiperazino, 191-2° (heptane); H, H, H, N'-ethylpiperazino, 175°; H, H, H, CH₂CH₂CH₂CHMe₂, 129-30°; H, Ph, H, nonyl, 126-38°; H, H, H, decyl, 110-11°; H, H, H, cyclohexyl, 149-51°; H, H, H, benzyl, 196°; H, Me, H, CH₂C₆H₄Me-4, 211°; H, H, H, CH₂CH₂Ph, 197-8° (HCl salt m. 231-4°); H, H, H, CH₂CH₂NMe₂, 164-5°; H, H, H, CH₂CH₂NEt₂, 146-7°; H, Me, H, CH₂CH(OEt)₂, 129-30°; H, H, H, CH₂CH₂CH(OEt)₂, 120-1°; H, H, H, CO₂Me, decompd. 265-70°; H, H, H, furyl, 154°; H, H, Me, CH₂CH(OEt)₂, 127-9°; H, Me, Me, CH₂CH(OEt)₂, 155°; H, H, Me, CH₂CH₂CH(OEt)₂, 87-9°; H, H, Et, CO₂Me, 204°; H, H, H, morpholino, 215°; H, Me, H, nonyl, 110-13°; H, Me, H, CH₂CH₂Ph, 208-9°. In another example 1.7 g. I, 3 g. pyrrolidine, and 35 cc. 95% EtOH were heated in a bomb at 130° 6.5 hrs., evapd., the residue dissolved in H₂O at pH 2 by adding 1:1 HCl, filtered from tar, adjusted to pH 10 and filtered to give 1.7 g. I (R¹, R², R³ = H, R⁴ = pyrrolidino), m. 263-5°. The following compds. were prepd. similarly (R¹, R², R³, R⁴, and m.p. given): H, H, H, H, 2905°; H, Me, H, CH₂CH₂CH₂OMe, 188-9°; H, Me, H, 2-pyridylmethyl, 215-16°; H, Me, H, 3,4,5-trimethoxybenzyl, 216-17°; H, Me, H, CH₂C₆H₄Me-3, 184-5° (HCl salt m. 230-6°); H, H, H, 2-thenyl, 272-6°; H, H, H, CH₂C₆H₄Cl-2, 220-2°; H, H, H, CH₂C₆H₄Me-4, 203-5°; H, H, Me, benzyl, 228-30°; H, H, H, CH₂C₆H₄Cl-4, 205-6°; H, H, H, CH₂C₆H₄OMe-4, 236-9°; H, H, Me, nonyl, 105-6°; H, H, Me, benzyl, 178-80°; H, H, H, CH₂C₆H₄Me-2, 259-61°; H, H, H, 2-pyridyl, 184-6°; H, H, CH₂CH₂OH, CH₂CH₂OH, 196-8°; H, Pr, H, nonyl, 94-6°; Me, H, H, nonyl, West-(HCl salt m. 129-30°); Me, Me, H, benzyl, 147-8°; Me, H, H, 4-methylpiperazino, decompd. 190-210° then m. 233-8°; H, Pr, H, benzyl, 161-2°; H, Pr, H, 4-ethylpiperazino, 121°; H, H, H, 4-isopropylpiperazino, 178-9°; H, H, H, 4-propylpiperazino, 172-4°; H, H, H, 4-carbethoxypiperazino, 204-5°; H, H, H, 4-(2hydroxyethyl)piperazino, 176-7°; H, H, H, 4-butylpiperazino, 171-2°; H, H, H, 3,4,5-trimethylpiperazino, 206-7°; H, H, H, 4-ethylpiperazino, 225-30°; H, Me, H, CH₂C₆H₄OMe-4, 189-91°; H, Me, H, CH₂CH₂CH₂OCHMe₂, 130-40°; H, Me, Me, Pr, 123-4°; H, Me, H, 4-propylpiperazino, 194-6°; H, Me, H, PhCH₂CH₂, 208-9° (HCl salt m. 112-16°); H, Me, H, CH₂C₆H₄Cl-4, 234-5°; H, Me, Me, CH₂Ph, 218-19°; H, Me, H, 2-thenyl, 214-15°; H, Me, H, CH₂C₆H₄Cl-2, 219-22°; H, Me, H, α-furyl, 195-7°. Other pyrrolo[2,3-d]pyrimidines prepd. were (substituents and m.p. given): 4-octyloxy, 107-9°; 4-octylthio, 111-12°; 2,4-Me(Me₂NCH₂CH₂O), 201-3°; and 2-methyl, 179-80°. The products have hypotensive, muscle relaxant, hypnotic, and anticonvulsant effects. They are toxic at approx. 100 mg./kg. In dogs at 0.5 to 4 mg./kg. they produce a systolic drop of 5-45 mm. lasting up to 1.5 hrs. EtO₂CCH(CN)CH₂CH(OEt)₂ (11.4 g.) in 25 cc. EtOH was mixed with 4.3 g. MeC(NH₂):NH₄Cl and 1.15 g. Na in 25 cc. EtOH, refluxed 6 hrs., evapd., adjusted to pH 5 with AcOH and filtered to give an intermediate which in 100 cc. EtOH and 2 cc. concd. H₂SO₄ was refluxed 6 hrs., cooled, and filtered to give 4-hydroxy-2-methylpyrrolo[2,3-d]pyrimidine. To 5.8 g. II in 40 cc. NaH-dried HCONMe₂ at

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15° was added 0.95 g. NaH, the reaction mixt. held at room temp. 6-7 hrs., cooled to 5°, and 6.2 g. MeI added. After 24 hrs. at room temp. and 3-4 hrs. at 45°, 40 cc. H₂O was added and the reaction mixt. cooled overnight and filtered to give 4.1 g. 7-methyl-4-chloropyrrolo[2,3-d]pyrimidine.

IT ***94966-89-9*** , 7H-Pyrrolo[2,3-d]pyrimidine, 4-(nonylamino)-2-phenyl-
(prepn. of)

L3 ANSWER 30 OF 30 HCAPLUS COPYRIGHT 2004 ACS

ED Entered STN: 22 Apr 2001

ACCESSION NUMBER: 1962:46024 HCAPLUS

DOCUMENT NUMBER: 56:46024

ORIGINAL REFERENCE NO.: 56:8712e-i,8713a-c

TITLE: 2-Alkyl(aryl)- and 2,7-dimethyl-4-substituted
amino-pyrrolo[2,3-d]pyrimidines

AUTHOR(S): West, R. A.; Beauchamp, L.

CORPORATE SOURCE: Wellcome Research Labs., Tuckahoe, NY

SOURCE: Journal of Organic Chemistry (1961), 26, 3809-12

CODEN: JOCEAH; ISSN:0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 56:46024

AB Amidines condensed with Et α -cyano- γ,γ -diethoxybutyrate (I) gave pyrimidine derivs. which were further cyclized to 4-hydroxypyrrolo[2,3-d]pyrimidines. The various 4-chloropyrrolopyrimidines resulting from treatment of the OH compds, with PCl₃ reacted readily with amines to yield 4-substituted amino derivs. having pharmacol. activity. Acetamidine-HCl (4.7 g.) left 1 hr. at room temp. with 75 ml. soln. of 0.1 mole NaOEt, the NaCl removed, the filtrate refluxed 5 hrs. with I, evapd., the residue dissolved in 80 ml. cold H₂O, the pyrimidine pptd. at pH 7, cooled overnight, and dried gave 10.8 g. 2-methyl-4-hydroxy-5-(β,β -diethoxyethyl)pyrimidine (II), decompd. at 253-60° to a dark oil. The following 4-hydroxy-6-amino-5-(β,β -diethoxyethyl)pyrimidines were thus obtained (2-substituent, % yield, m.p. given): Me, 89, 249-50°; Et, 93, 238-5°; Pr, 77, 207-9°; Ph, 71, 174-6°. II (4.5 g.) refluxed 2 hrs. with 2 ml. concd. H₂SO₄ in 110 ml. 95% alc., an equal vol. of H₂O added, and the mixt. chilled overnight gave 2.1 g. 2-methyl-4-hydroxypyrrolo[2,3-d]pyrimidine (III), no m.p. below 300°. III (25 g.) suspended in 175 ml. POCl₃ refluxed 45 min., excess POCl₃ evapd. at 55-60° in vacuo, the oil dropped slowly into 1l. ice H₂O, the product extd. with Et₂O, dried, and evapd. gave 23.2 g. 2-methyl-4-chloropyrrolo[2,3-d]pyrimidine (IV). IV (5 g.) added to 1.9 g. Na-OMe in 50 ml. alc. at 5-10°, to this added 2.4 ml. MeI, the mixt. warmed 2 days at 40-5° in a sealed flask, the solvent evapd., the solid triturated with H₂O, and filtered gave 4 g.

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2,7-dimethyl-4-chloropyrrolo[2,3-d]pyrimidine. The following pyrrolo[2,3-d]pyrimidines were thus obtained (2, 7, 4 substituents, % yield, and m.p. given): Me, H, OH, 76, no m.p. to 320°; Et, H, OH, 85, no m.p. to 320°; Pr, H, OH, 85, no m.p. to 320°; Ph, H, OH, 93, no m.p. to 320°; H, Me, Cl, 75, 130°; Me, H, Cl, 83, 205-7°; Me, Me, Cl, 70, 121-2°; Et, H, Cl, 72, 125-7°; Pr, H, Cl, 82, 129-30°; Ph, H, Cl, 80, 225-6°. Method A.

2-Phenyl-4-chloropyrrolo[2,3-d]pyrimidine (1 g.) added to 35 ml. H₂O contg. 0.9 g. K₂CO₃ and 1 g. PhCH₂NH₂ and cooled overnight gave 1.2 g. crude

2-phenyl-4-benzylaminopyrrolo[2,5-d]pyrimidine. The product was recrystd. from C₆H₆heptane. Method B. IV (2.06 g.) and 6.04 g. o-anisidine refluxed 1.5 hrs. with 17 ml. HCONMe₂, chilled overnight with an equal vol. of H₂O, filtered, and dried gave 3.1 g.

2-methyl-4-(2-methoxyanilino)pyrrolo[2,3-d]pyrimidine, m. 255-6° (decompn.). IV (2 g.) suspended in 40 ml. concd. NH₄OH heated 4.5 hrs. at 145° in a bomb, evapd., and the product collected gave 1.3 g. 2-methyl-4-aminopyrrolo[2,3-d]pyrimidine, m. 305-7° (decompn.).

The following 4substituted aminopyrrolo[2,3-d]pyrimidines were thus obtained (2, 7, 3 substituents, m.p., and % yield given): H, Me, NH₄Et, 157-8°, 88; Me, H, NH₄Et, 189-90°, 89; Me, H, CMePr, 124-5°, 93; Me, H, 2-thenylamino, 214-15°, 91; Me, H, NHC₆H₄Me-m, 248°, 98; Me, Me, NHCH₂Ph, 147-8°, 90; Me, H, NHCH₂Ph, 223-4°, 93; Et, H, NHCH₂Ph, 183°, 90; Pr, H, NHCH₂Ph, 170-1°, 92; Ph, H, NHCH₂Ph, 162-4°, 92. The ultraviolet spectral data of pyrrolo[2,3-d]pyrimidines and precursors were given in a table at pH 1.0 and pH 11.0. Some of the substituted amino compds, had pronounced pharmacol. effects in test animals including anticonvulsant, muscle relaxant, hypotensive and tranquilizer activities.

IT ***94304-61-7*** , 7H-Pyrrolo[2,3-d]pyrimidine, 4-(benzylamino)-2-phenyl-
(prepn. of)

IT ***92193-06-1*** , 7H-Pyrrolo[2,3-d]pyrimidine, 4-(ethylamino)-2-phenyl-
(spectrum of)
